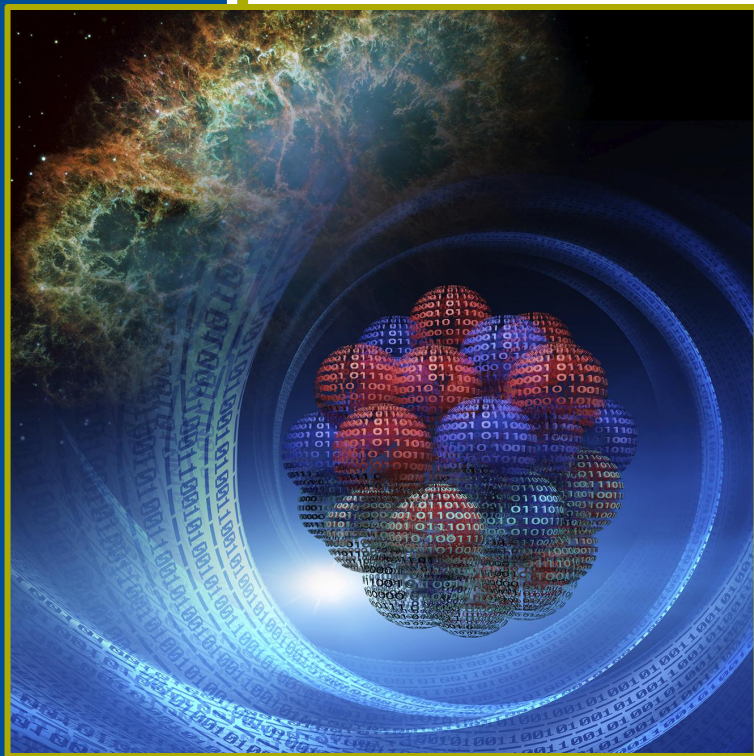




Andy Sproles, ORNL

Microscopic models of nuclear structure at scale

W. Ryssens

19th of March 2025



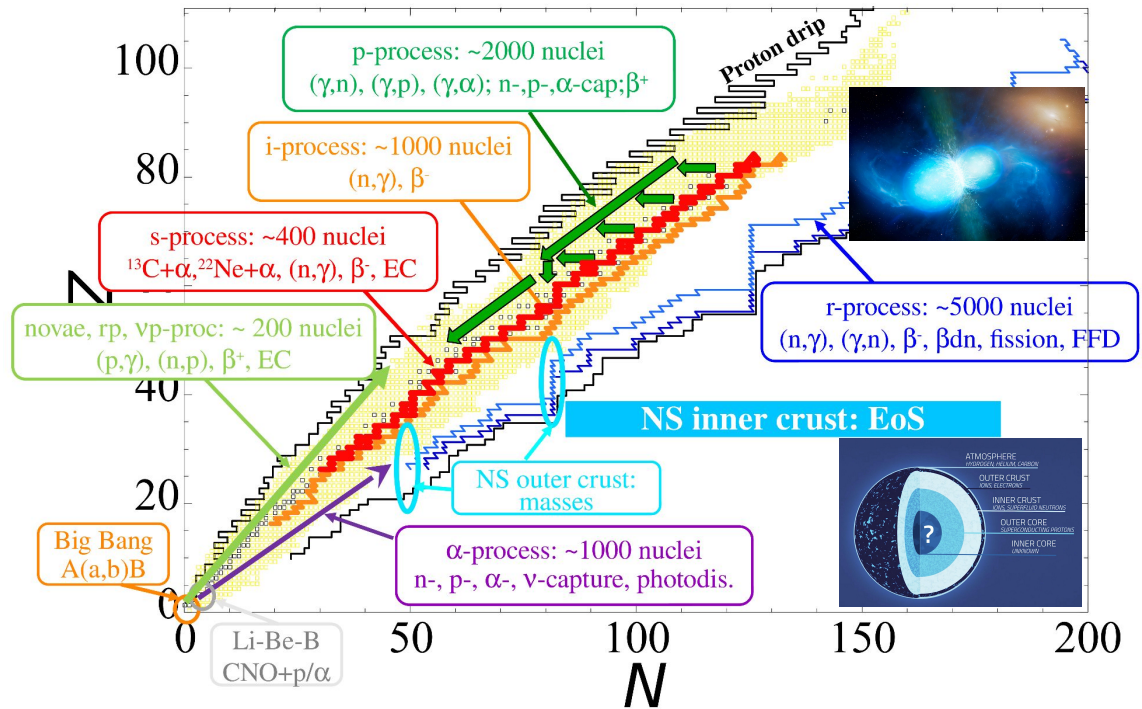
wryssens.com

wryssens@ulb.be

The nuclear chart and the processes traversing it

Extrapolations in

- nucleon number
- energy
- temperature
- density
-



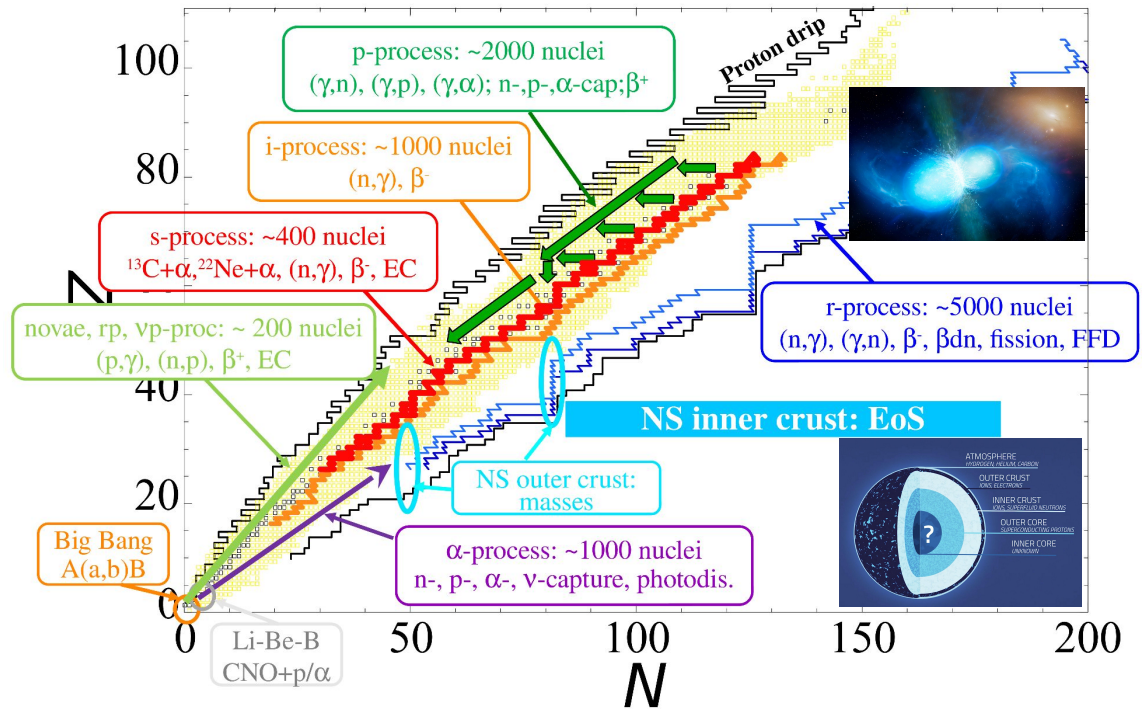
The nuclear chart and the processes traversing it

Extrapolations in

- nucleon number
- energy
- temperature
- density
-

and all of that for

- **~7000** nuclei
- **many** reactions



The nuclear chart and the processes traversing it

Extrapolations in

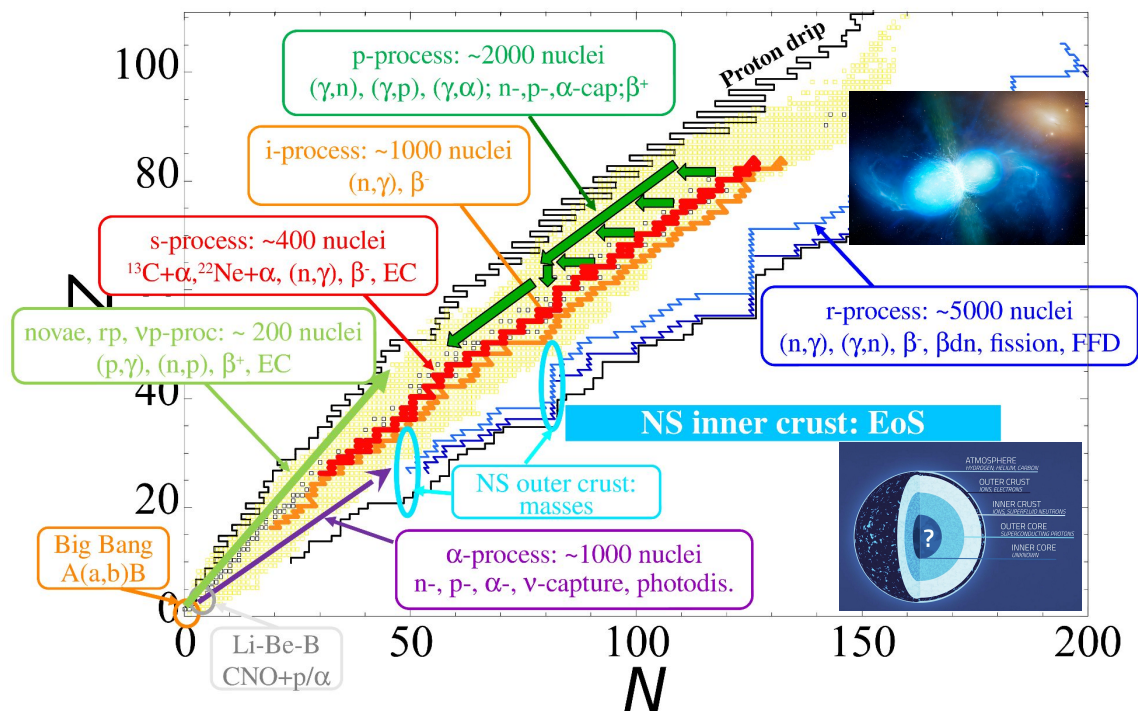
- nucleon number
- energy
- temperature
- density
-

and all of that for

- ~7000 nuclei
- many reactions

We need structure models that are

1. predictive....
2. but complete!

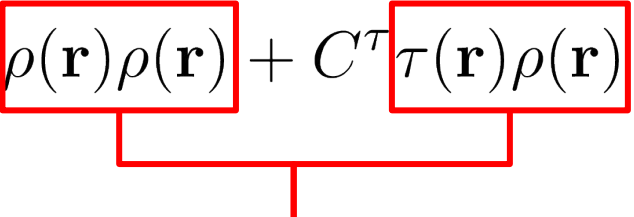


Skyrme **E**nergy **D**ensity **F**unctionals (**EDFs**)

$$E \sim \int d^3r \left[C^\rho \rho(\mathbf{r})\rho(\mathbf{r}) + C^\tau \tau(\mathbf{r})\rho(\mathbf{r}) + \dots \right]$$



Skyrme **E**nergy **D**ensity **F**unctionals (**EDFs**)

$$E \sim \int d^3r \left[C^\rho \boxed{\rho(\mathbf{r})\rho(\mathbf{r})} + C^\tau \boxed{\tau(\mathbf{r})\rho(\mathbf{r})} + \dots \right]$$


Local densities and currents of a wavefunction



Skyrme **E**nergy **D**ensity **F**unctionals (**EDFs**)

Coupling constants (~ **25** parameters) fitted to data

The diagram shows the Skyrme Energy Density Functional equation:
$$E \sim \int d^3r \left[C^\rho \rho(\mathbf{r})\rho(\mathbf{r}) + C^\tau \tau(\mathbf{r})\rho(\mathbf{r}) + \dots \right]$$
 Annotations include: a blue line connecting the coupling constants C^ρ and C^τ to the text 'Coupling constants (~ 25 parameters) fitted to data'; and a red bracket under the density and current terms $\rho(\mathbf{r})\rho(\mathbf{r})$ and $\tau(\mathbf{r})\rho(\mathbf{r})$ pointing to the text 'Local densities and currents of a wavefunction'.

Local densities and currents of a wavefunction



Skyrme **E**nergy **D**ensity **F**unctionals (**EDFs**)

Energy

Coupling constants (~ **25** parameters) fitted to data

$$E \sim \int d^3r \left[C^\rho \rho(\mathbf{r})\rho(\mathbf{r}) + C^\tau \tau(\mathbf{r})\rho(\mathbf{r}) + \dots \right]$$

Local densities and currents of a wavefunction

The diagram shows the Skyrme Energy Density Functional equation. The energy E is represented by a magenta box. The coupling constants C^ρ and C^τ are in blue boxes, and the density and current terms $\rho(\mathbf{r})\rho(\mathbf{r})$ and $\tau(\mathbf{r})\rho(\mathbf{r})$ are in red boxes. A blue line connects the coupling constants to the text 'Coupling constants (~ 25 parameters) fitted to data'. A red line connects the density and current terms to the text 'Local densities and currents of a wavefunction'. The equation is enclosed in large square brackets.

Skyrme **E**nergy **D**ensity **F**unctionals (**EDFs**)

Energy

Coupling constants (~ 25 parameters) fitted to data

$$E \sim \int d^3r \left[C^\rho \rho(\mathbf{r})\rho(\mathbf{r}) + C^\tau \tau(\mathbf{r})\rho(\mathbf{r}) + \dots \right]$$

Local densities and currents of a wavefunction

The diagram illustrates the Skyrme Energy Density Functional (EDF) equation. The energy E is represented by a pink box. The coupling constants C^ρ and C^τ are highlighted with blue boxes, indicating they are parameters fitted to data. The local densities and currents $\rho(\mathbf{r})\rho(\mathbf{r})$ and $\tau(\mathbf{r})\rho(\mathbf{r})$ are highlighted with red boxes, indicating they are properties of the wavefunction. The equation is shown as $E \sim \int d^3r [C^\rho \rho(\mathbf{r})\rho(\mathbf{r}) + C^\tau \tau(\mathbf{r})\rho(\mathbf{r}) + \dots]$.

Progress?

1. more physics in the wavefunction

Skyrme **E**nergy **D**ensity **F**unctionals (**EDFs**)

Energy

Coupling constants (~ **25** parameters) fitted to data

$$E \sim \int d^3r \left[C^\rho \rho(\mathbf{r})\rho(\mathbf{r}) + C^\tau \tau(\mathbf{r})\rho(\mathbf{r}) + \dots \right]$$

Local densities and currents of a wavefunction

Progress?

1. more physics in the wavefunction
2. more (pseudo-) observables simultaneously
“more” = both scale and diversity!

Skyrme **E**nergy **D**ensity **F**unctionals (**EDFs**)

Energy

Coupling constants (~ **25** parameters) fitted to data

$$E \sim \int d^3r \left[C^\rho \rho(\mathbf{r})\rho(\mathbf{r}) + C^\tau \tau(\mathbf{r})\rho(\mathbf{r}) + \dots \right]$$

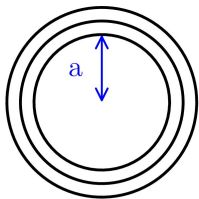
Local densities and currents of a wavefunction

Progress?

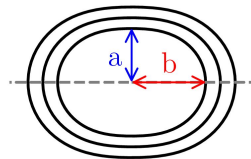
1. more physics in the wavefunction
2. more (pseudo-) observables simultaneously
“more” = both scale and diversity!
3. search for a “better” EDF form

Large-scale models in 1-2 dimensions

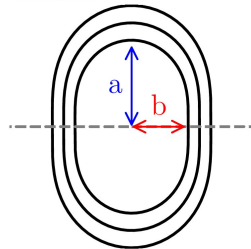
Spherical



Prolate



Oblate



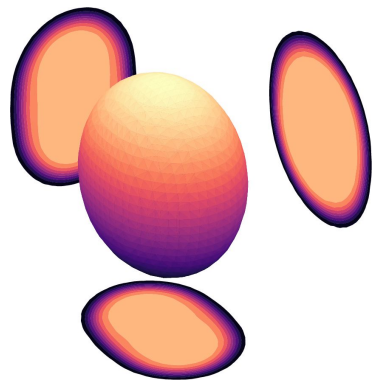
One DOF: β_{20}

Nuclear deformation

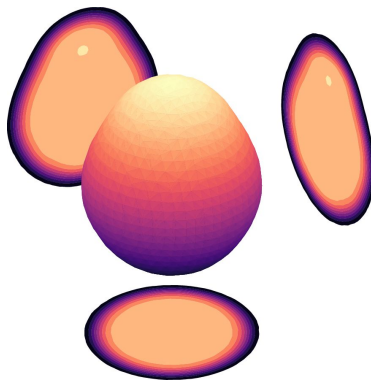
- larger variational space
- shape DOF characterized by multipole moments
- capture correlations at modest CPU cost
- intuitive interpretation

Large-scale models in 1-2-**3** dimensions

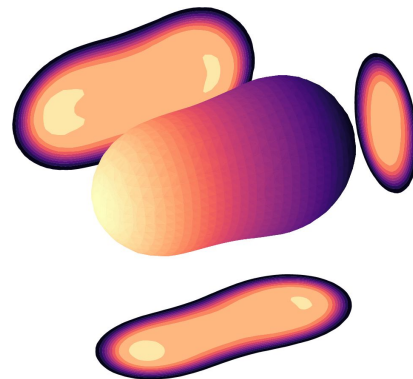
β_{20}, β_{22} or β_2, γ



β_{20}, β_{30}



β_{20}, β_{22} **and** β_{30}



Nuclear deformation

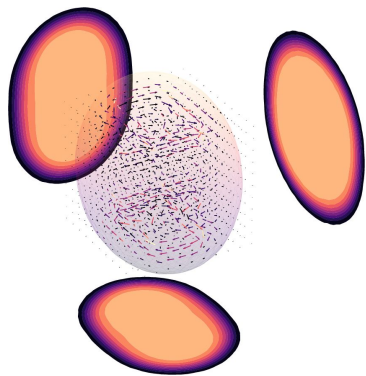
- larger variational space
- shape DOF characterized by multipole moments
- capture correlations at modest CPU cost
- intuitive interpretation

More general configurations

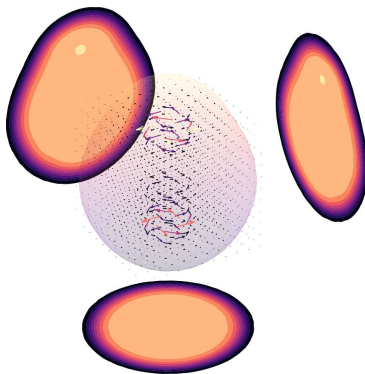
- triaxial shapes
- reflection asymmetry
- elongated shapes

Large-scale models in 1-2-**3** dimensions

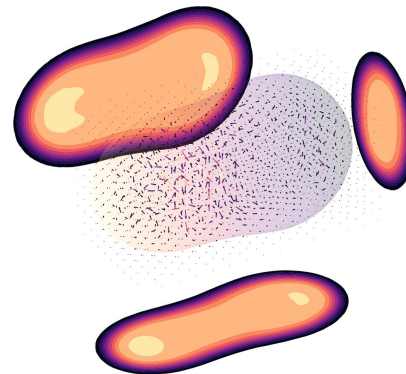
β_{20}, β_{22} or β_2, γ



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β_{20}, β_{22} **and** β_{30}



Nuclear deformation

- larger variational space
- shape DOF characterized by multipole moments
- capture correlations at modest CPU cost
- intuitive interpretation

More general configurations

- triaxial shapes
- reflection asymmetry
- elongated shapes
- spin densities and currents

Brussels-Skyrme-on-a-Grid: BSkG

BSkG1

- fitted to 2457 masses
- fitted to 884 charge radii
- includes triaxial deformation

BSkG1: G. Scamps et al., EPJA **57**, 333 (2021).
BSkG2: W. Ryssens et al., EPJA **58**, 246 (2022).
W. Ryssens et al., EPJA **59**, 96 (2023).
BSkG3: G. Grams et al., EPJA **59**, 270 (2023).
BSkG4: G. Grams et al., arXiv:2411.08007 (2024).

Rms σ	BSkG1	BSkG2	BSkG3	BSkG4
Masses [MeV]	0.741			
S_n [MeV]	0.466			
Radii [fm]	0.024			
Prim. barriers [MeV]				
Sec. barriers [MeV]				
Fission isomers [MeV]				
Max. NS mass [$M_\odot$]				

Brussels-Skyme-on-a-Grid: BSkG

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- includes triaxial deformation

Rms σ	BSkG1	BSkG2	BSkG3	BSkG4
Masses [MeV]	0.741	0.678		
S_n [MeV]	0.466	0.500		
Radii [fm]	0.024	0.027		
Prim. barriers [MeV]	0.88	0.44		
Sec. barriers [MeV]	0.87	0.47		
Fission isomers [MeV]	1.0	0.49		
Max. NS mass [$M_\odot$]				

BSkG2

- complete time-reversal breaking
- fit to 45 reference fission barriers
+ 28 fission isomers

Brussels-Skyme-on-a-Grid: BSkG

BSkG1

- fitted to 2457 masses
- fitted to 884 charge radii
- includes triaxial deformation

Rms σ	BSkG1	BSkG2	BSkG3	BSkG4
Masses [MeV]	0.741	0.678	0.631	
S_n [MeV]	0.466	0.500	0.442	
Radii [fm]	0.024	0.027	0.024	
Prim. barriers [MeV]	0.88	0.44	0.33	
Sec. barriers [MeV]	0.87	0.47	0.51	
Fission isomers [MeV]	1.0	0.49	0.34	
Max. NS mass [$M_\odot$]	1.8	1.8	2.3	

BSkG2

- complete time-reversal breaking
- fit to 45 reference fission barriers + 28 fission isomers

BSkG3

- extended Skyrme EDF form
- supports massive neutron stars

BSkG1: G. Scamps et al., EPJA **57**, 333 (2021).
BSkG2: W. Ryssens et al., EPJA **58**, 246 (2022).
W. Ryssens et al., EPJA **59**, 96 (2023).
BSkG3: G. Grams et al., EPJA **59**, 270 (2023).
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Brussels-Skyme-on-a-Grid: BSkG

BSkG1: G. Scamps et al., EPJA **57**, 333 (2021).
BSkG2: W. Ryssens et al., EPJA **58**, 246 (2022).
W. Ryssens et al., EPJA **59**, 96 (2023).
BSkG3: G. Grams et al., EPJA **59**, 270 (2023).
BSkG4: G. Grams et al., EPJA **61**, 35 (2024).

BSkG1

- fitted to 2457 masses
- fitted to 884 charge radii
- includes triaxial deformation

BSkG4

- pairing reproduces advanced INM calculations
- ideal for TD simulations in NS crust

Rms σ	BSkG1	BSkG2	BSkG3	BSkG4
Masses [MeV]	0.741	0.678	0.631	0.633
S_n [MeV]	0.466	0.500	0.442	0.402
Radii [fm]	0.024	0.027	0.024	0.025
Prim. barriers [MeV]	0.88	0.44	0.33	0.36
Sec. barriers [MeV]	0.87	0.47	0.51	0.53
Fission isomers [MeV]	1.0	0.49	0.34	0.33
Max. NS mass [$M_\odot$]	1.8	1.8	2.3	2.3

BSkG2

- complete time-reversal breaking
- fit to 45 reference fission barriers + 28 fission isomers

BSkG3

- extended Skyrme EDF form
- supports massive neutron stars

Investment in computing

MOCCa

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```

Density functional theory with MOCCa

- nonlinear optimisation problem
- algorithms for speed and robustness
- open-source later this year

Investment in computing

MOCCa

```
      ; ,  
    ) ; ( (  
  ( ( ) ) ;  
    , - " " " - .  
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(( _ |           |  
  ' - \           /  
    ' . - - - . '
```

Density functional theory with MOCCa

- nonlinear optimisation problem
- algorithms for speed and robustness
- open-source later this year

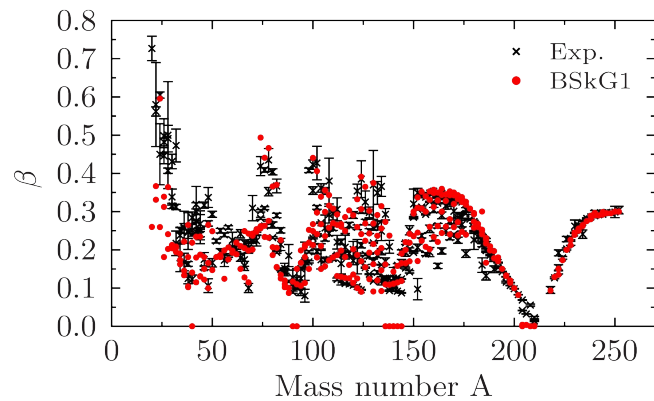
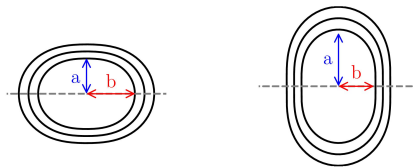


Raw computing power

- CÉCI & VSC: academic support in Belgium
- TIER-1 resources by Cenaero
 - Lucia - ranked 388th - our development workhorse
- TIER-0 resources by EuroHPC
 - MN 5 - ranked 11th - large scale fission
 - LUMI - ranked 8th - nuclear pasta

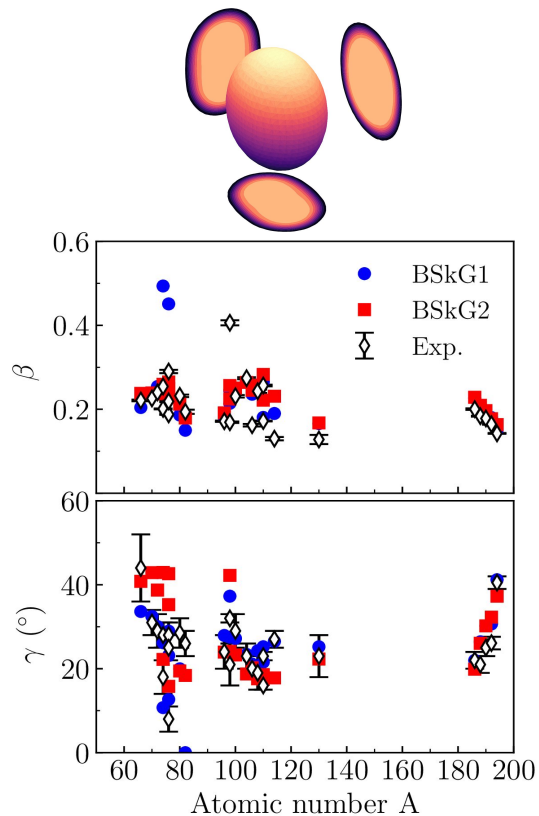
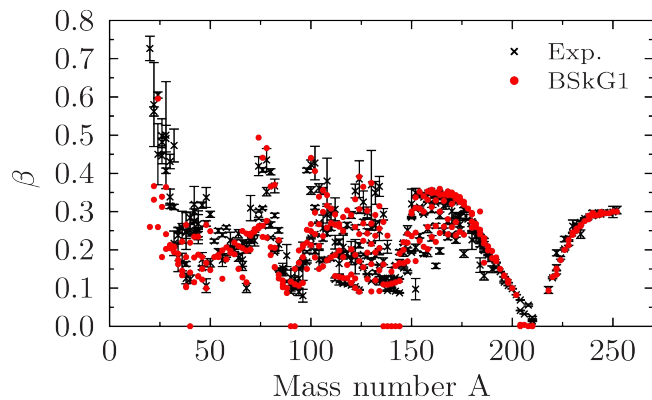
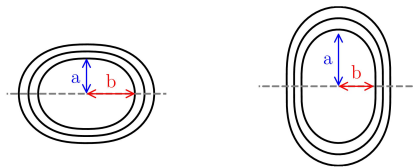
Deformations

“Ordinary” quadrupole deformation



Deformations

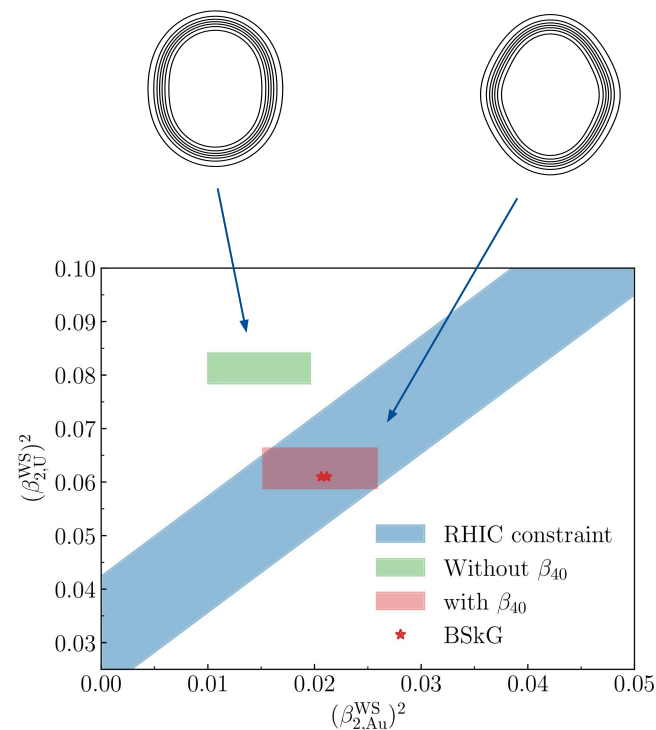
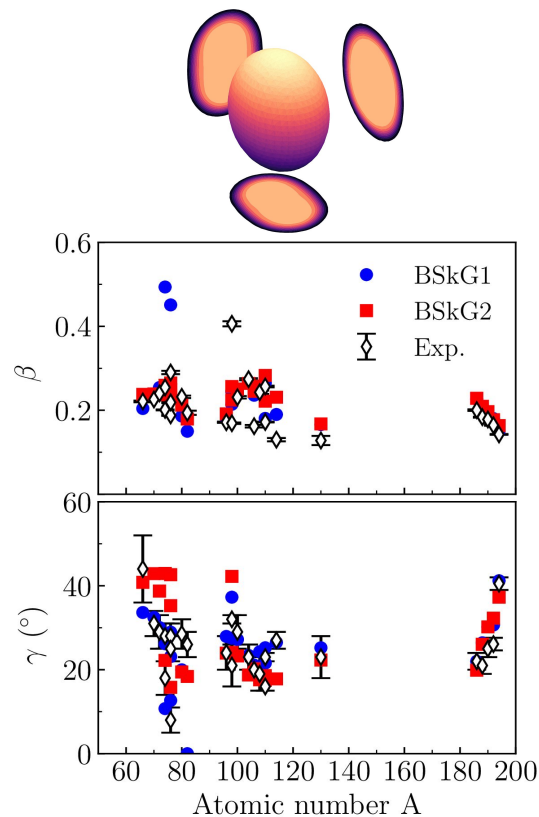
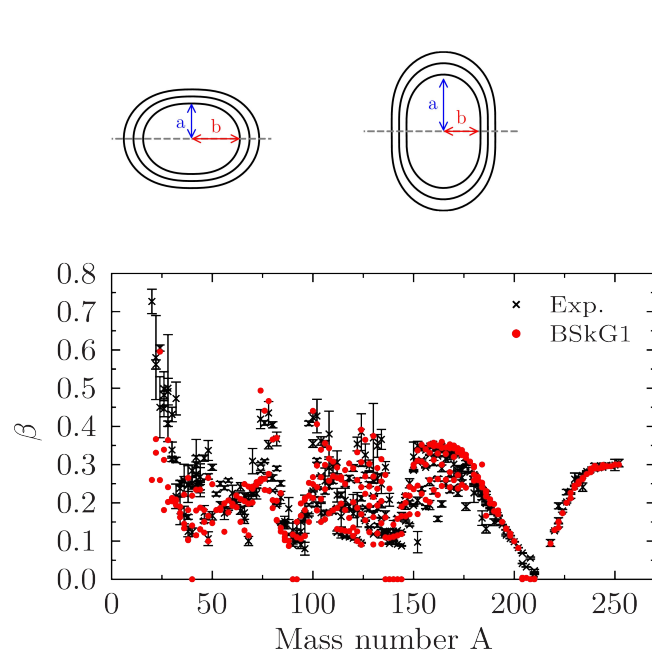
“Ordinary” quadrupole deformation ... and triaxial deformation ...



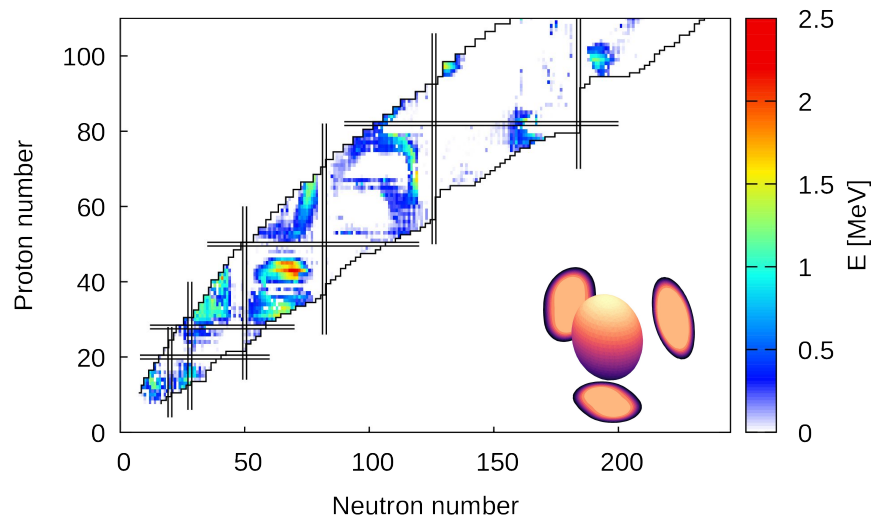
Deformations

“Ordinary” quadrupole deformation ... and triaxial deformation ...

... and even hexadecapole!



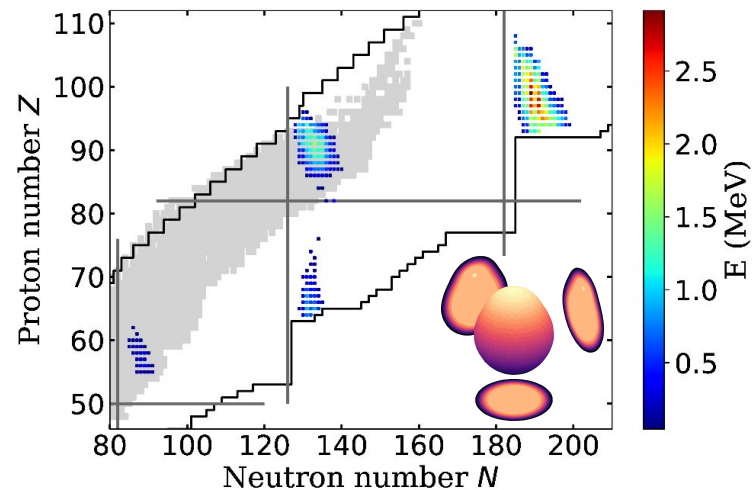
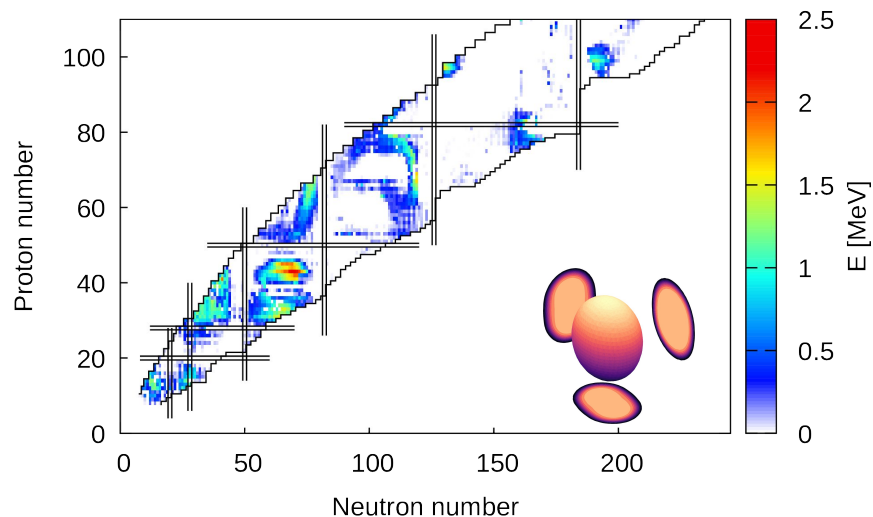
Masses



Triaxial deformation

- many nuclei are affected
- effects up to 2.5 MeV near $Z \sim 44$

Masses



Triaxial deformation

- many nuclei are affected
- effects up to 2.5 MeV near $Z \sim 44$

Reflection asymmetry

- small number of known nuclei affected
- Near $N=184$:
 - large effect up to 2.5 MeV
 - dripline modified
 - fission properties modified

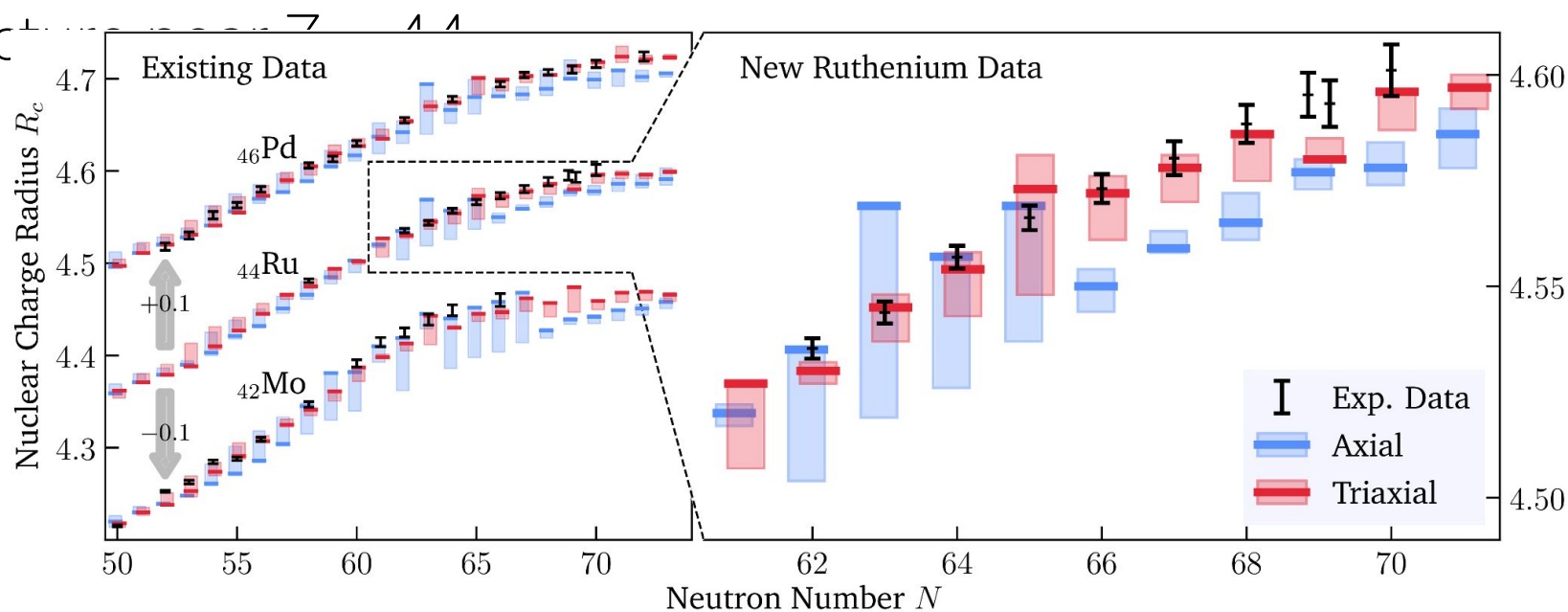
Structure near $Z \sim 44$

Triaxial deformation impacts

- spectroscopy
- patterns in masses
- existence and structure of isomers

M. Hukkanen, W.R. et al., PRC **107** (2023).
M. Hukkanen, W.R. et al., PRC **108** (2023).
M. Hukkanen, W.R. et al., PLB **856** (2024).
M. Stryczyk, W. R. et al., PLB **862** (2025).
B. Maass et al., arXiv:2503.07841 (2024).

Struc



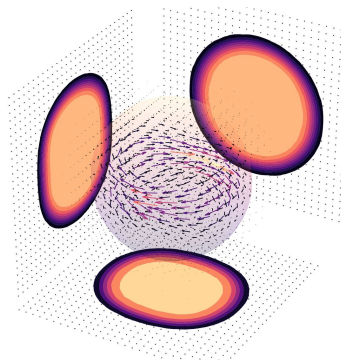
Triaxial deformation impacts

- spectroscopy
- patterns in masses
- existence and structure of isomers
- ! charge radii

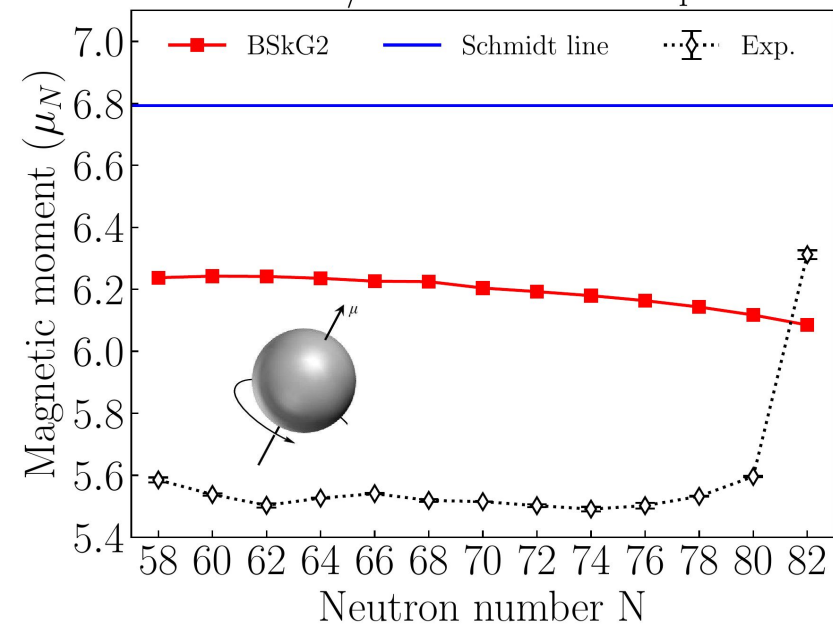
contrary to claims in the literature!

M. Hukkanen, W.R. et al., PRC **107** (2023).
M. Hukkanen, W.R. et al., PRC **108** (2023).
M. Hukkanen, W.R. et al., PLB **856** (2024).
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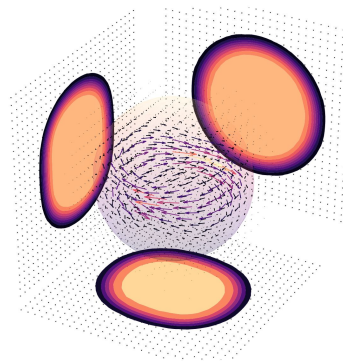
Time-odd channel



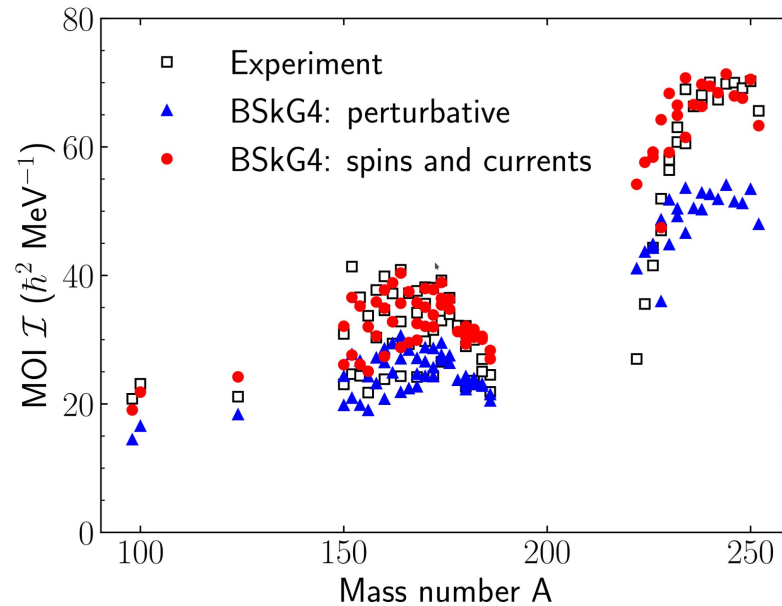
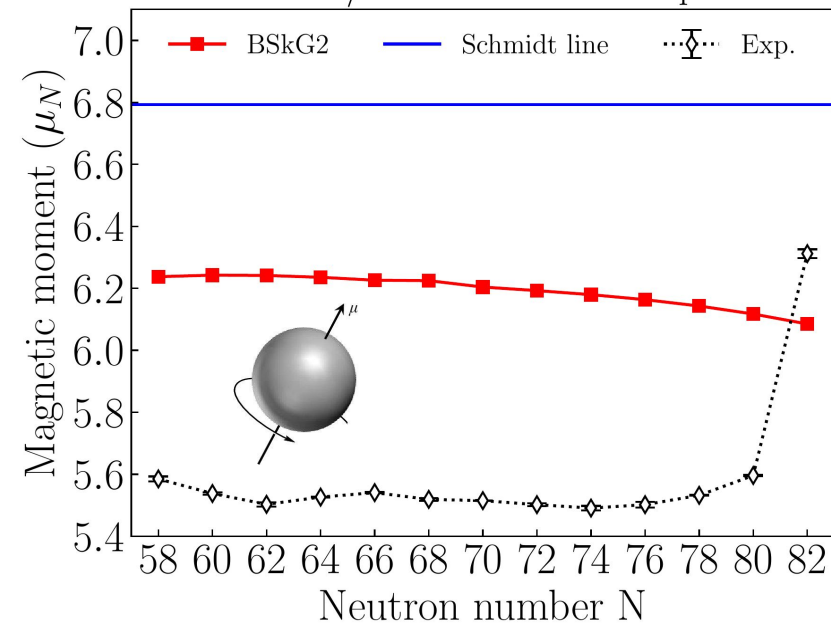
$J^\pi = 9/2^+$ states in In isotopes



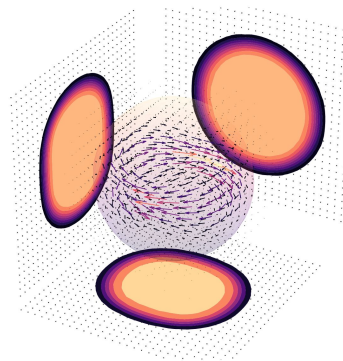
Time-odd channel



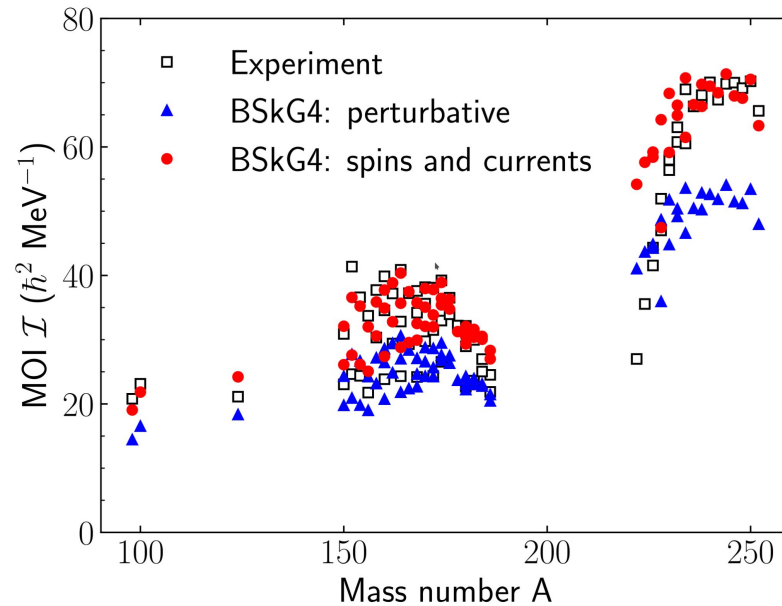
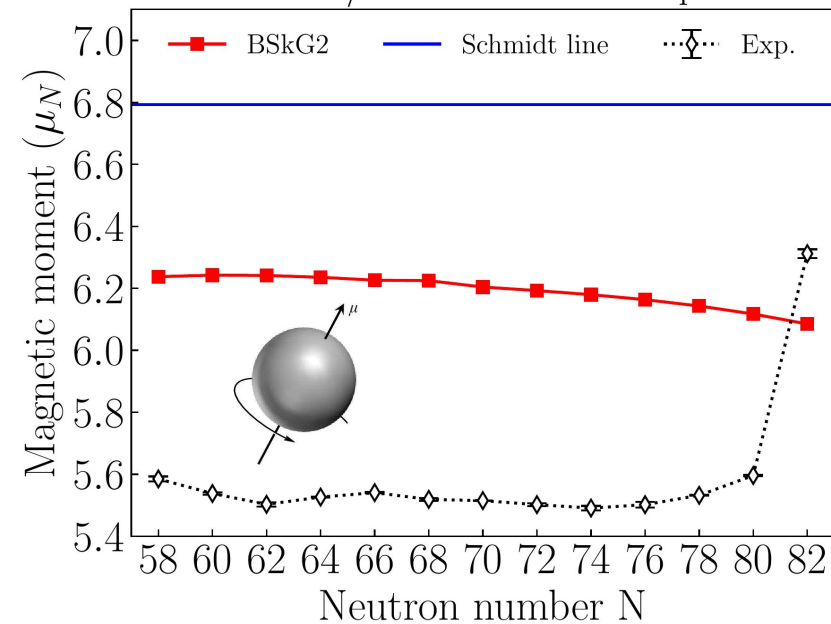
$J^\pi = 9/2^+$ states in In isotopes



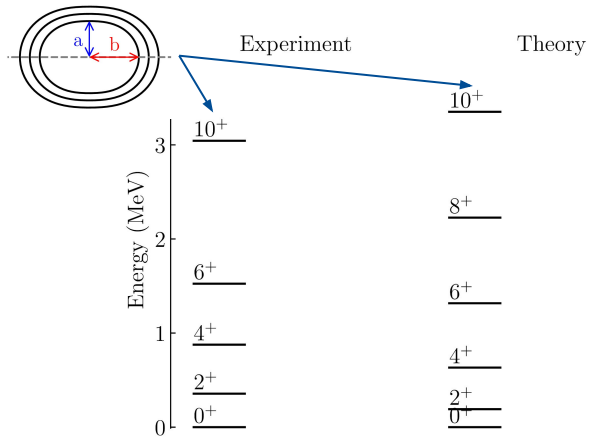
Time-odd channel



$J^\pi = 9/2^+$ states in In isotopes



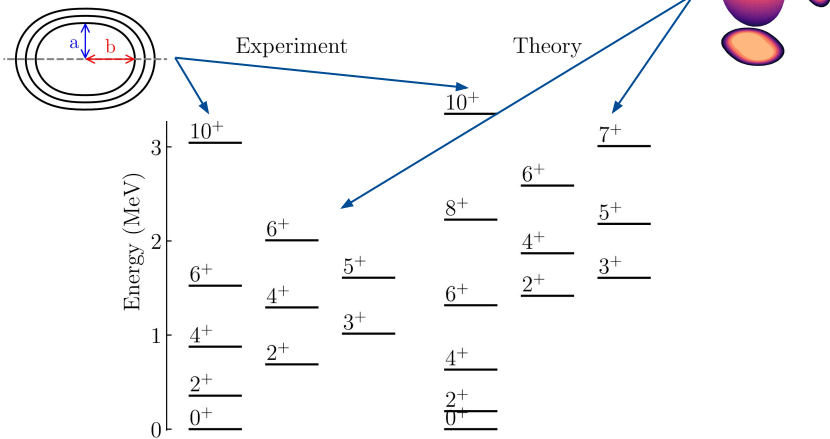
Nuclear level densities



Symmetries dictate NLDs

- larger collective enhancement

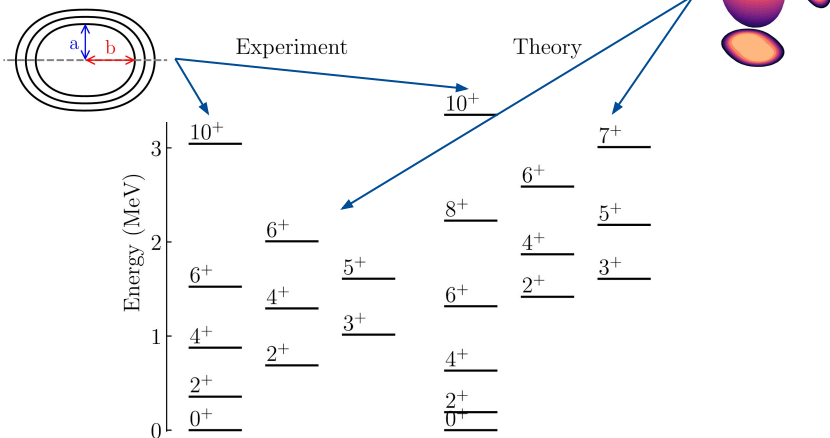
Nuclear level densities



Symmetries dictate NLDs

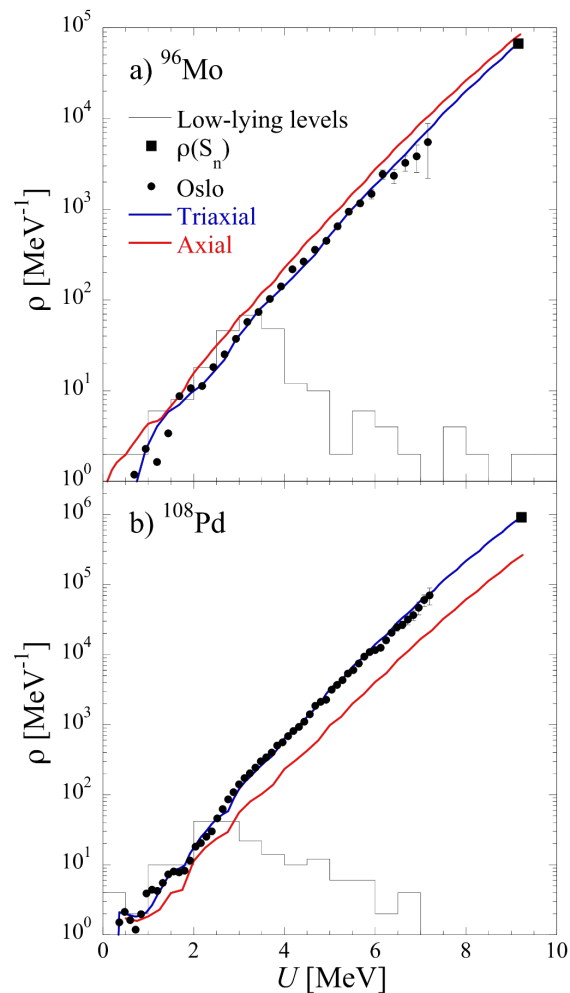
- larger collective enhancement

Nuclear level densities

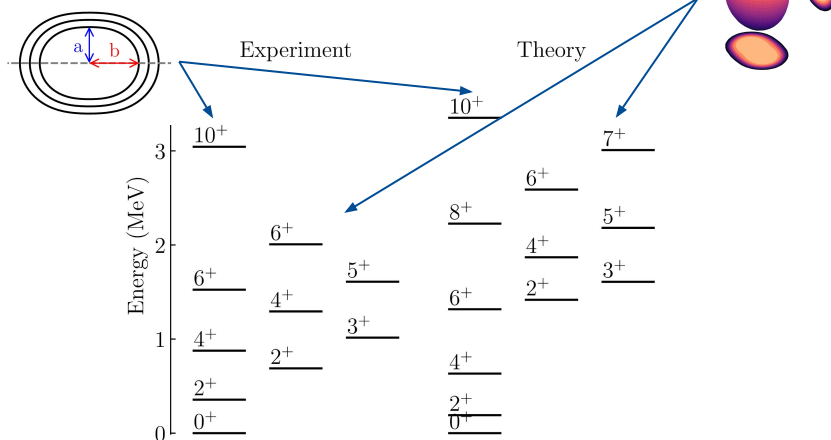


Symmetries dictate NLDs

- larger collective enhancement
- combinatorial calculation of NLDs
- ... but the story is not so simple!

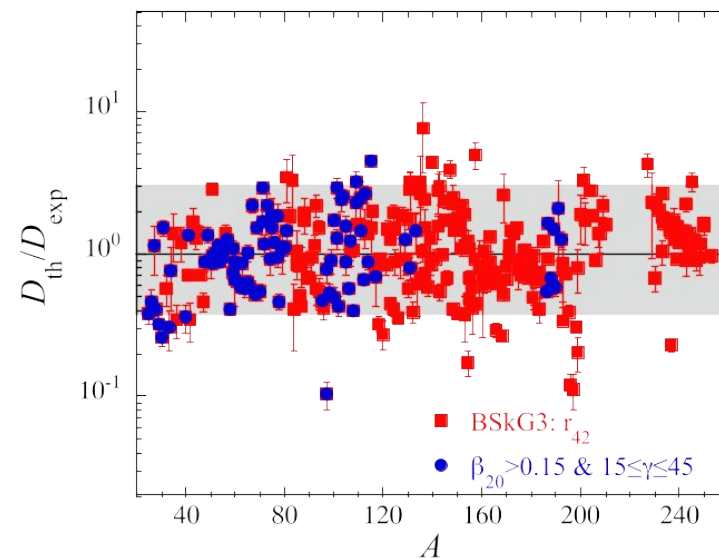


Nuclear level densities



Symmetries dictate NLDs

- larger collective enhancement
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- ... but the story is not so simple!



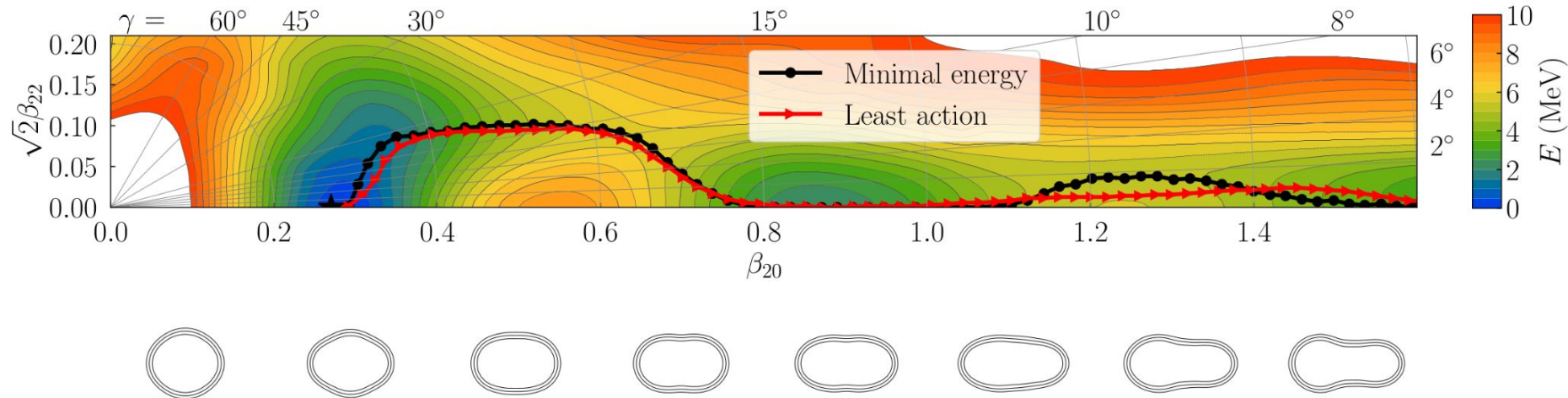
$$f_{\text{rms}} = \exp \left[\frac{1}{N_e} \sum_i^{N_e} (\ln r_i)^2 \right]^{1/2} = 1.96.$$

Fission barriers

W. R. et al., EPJA **59**, 96 (2023).

E. Flynn et al., PRC **105** (2022).

S. Bara et al. & A. Sánchez-Fernández et al., in preparation.

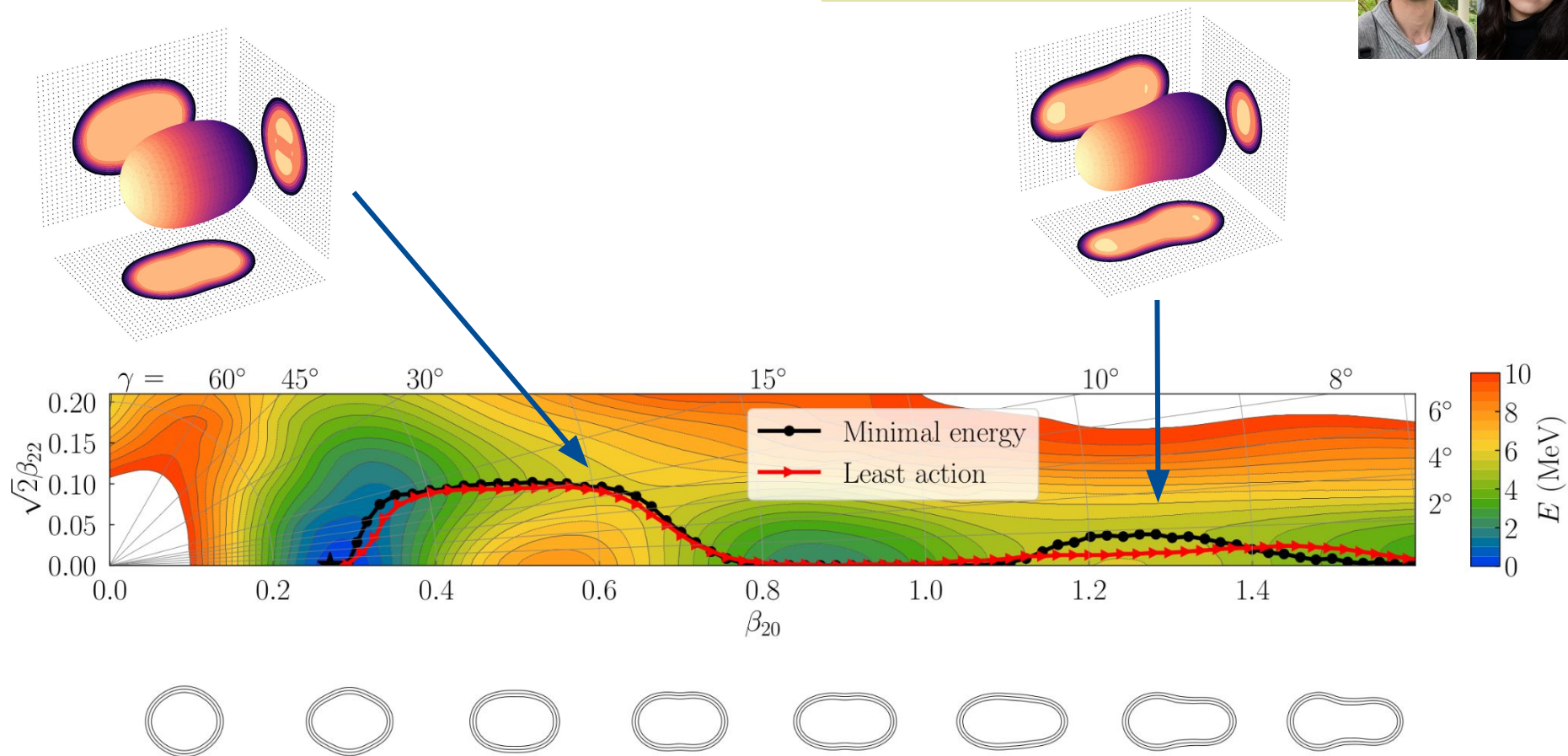


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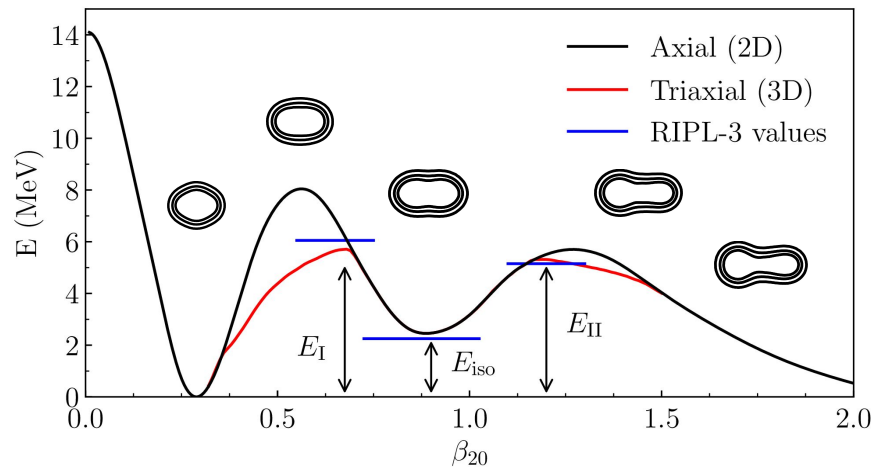


Fission

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E. Flynn et al., PRC **105** (2022).

S. Bara et al. & A. Sánchez-Fernández et al., in preparation.



Fission properties of 45 actinide nuclei

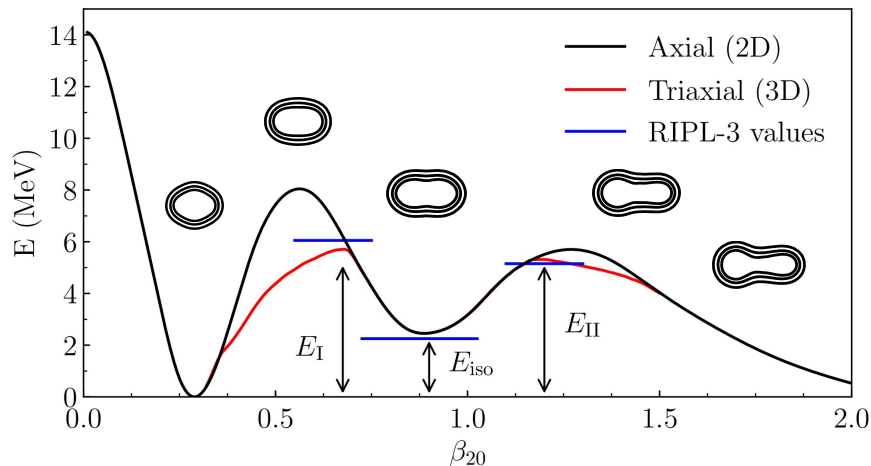
- includes odd-A and odd-odds
 - all inner barriers: triaxial
 - all outer barriers: octupole + triaxial
- ... even with consistent inertia's!

Fission

W. R. et al., EPJA **59**, 96 (2023).

E. Flynn et al., PRC **105** (2022).

S. Bara et al. & A. Sánchez-Fernández et al., in preparation.

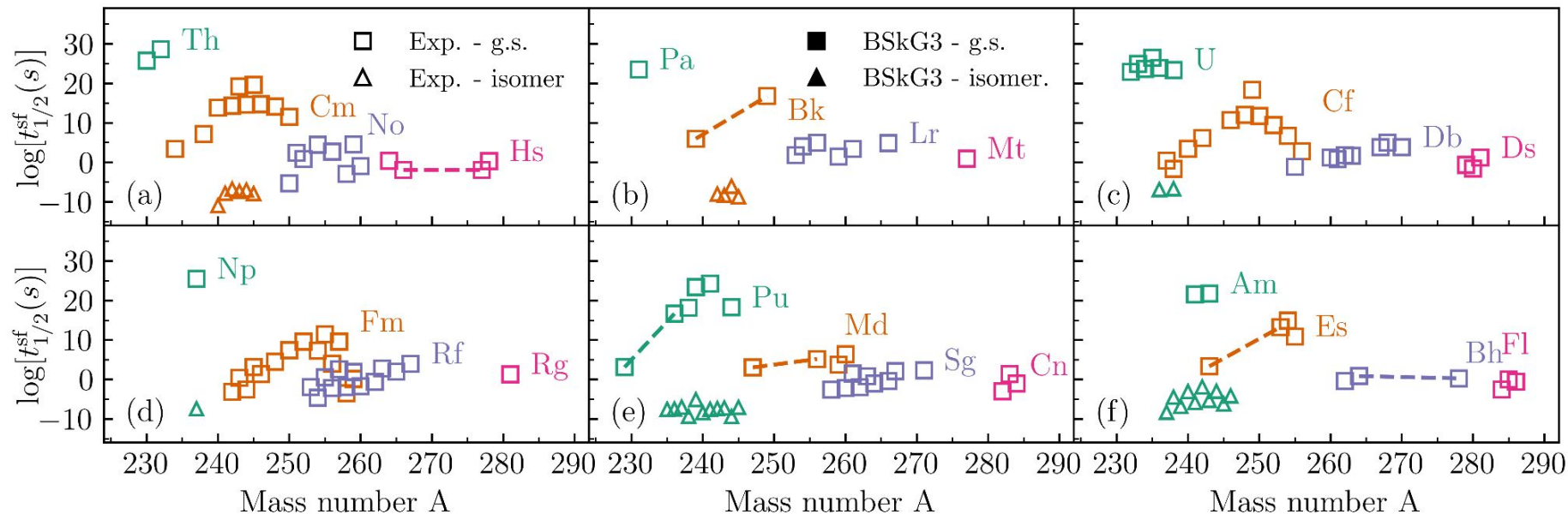


Fission properties of 45 actinide nuclei

- includes odd-A and odd-odds
- all inner barriers: triaxial
- all outer barriers: octupole + triaxial
- ... even with consistent inertia's!

Large-scale data generation

- poor-mans 3D coll. space: $\beta_{20}, \beta_{22}, \beta_{30}$
- odd nuclei through EFA
- pathfinding with PyNEB
- ✓ 1500/3000 nuclei ($Z > 78$)

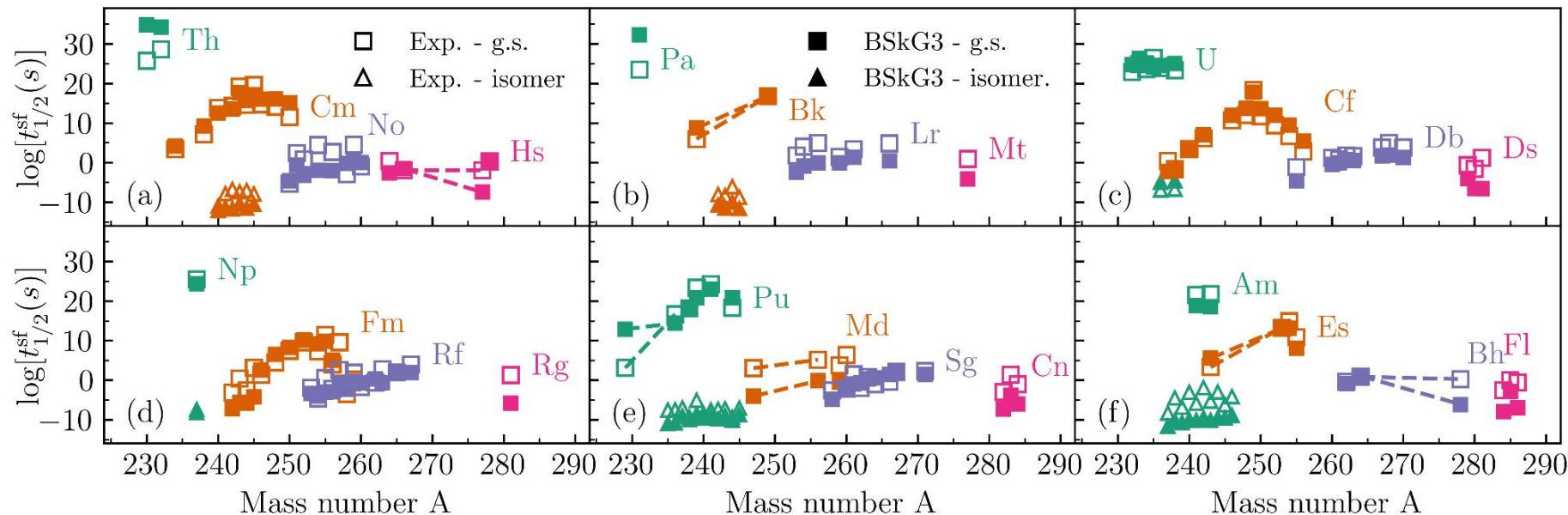


Spontaneous fission half-lives

Experimental data:

- 124 ground state half-lives
- 34 half-lives of isomeric states

... that span **> 40** orders of magnitude!



A. Sánchez-Fernández et al., in prep.

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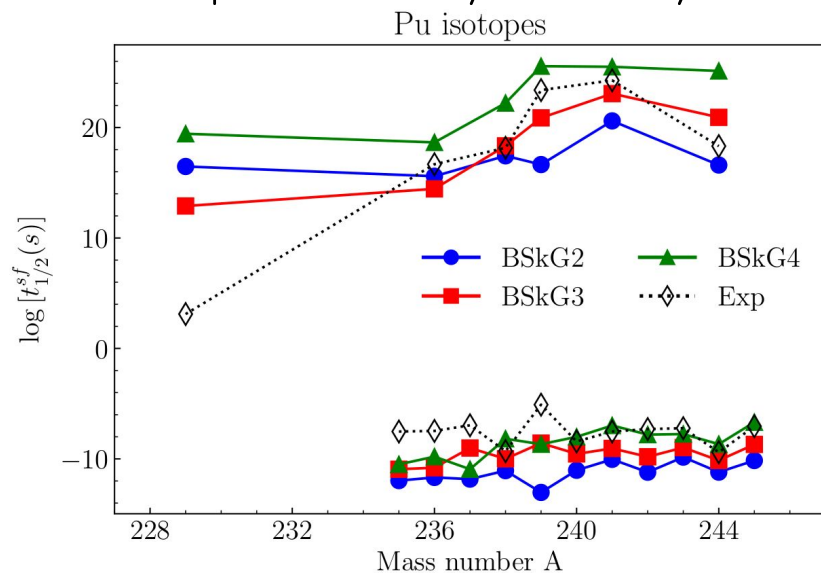
- 124 ground state half-lives
- 34 half-lives of isomeric states

... that span **> 40** orders of magnitude!

... at scale from microscopic models!

- comparable best mic-mac models
- ... without adjustable parameters!

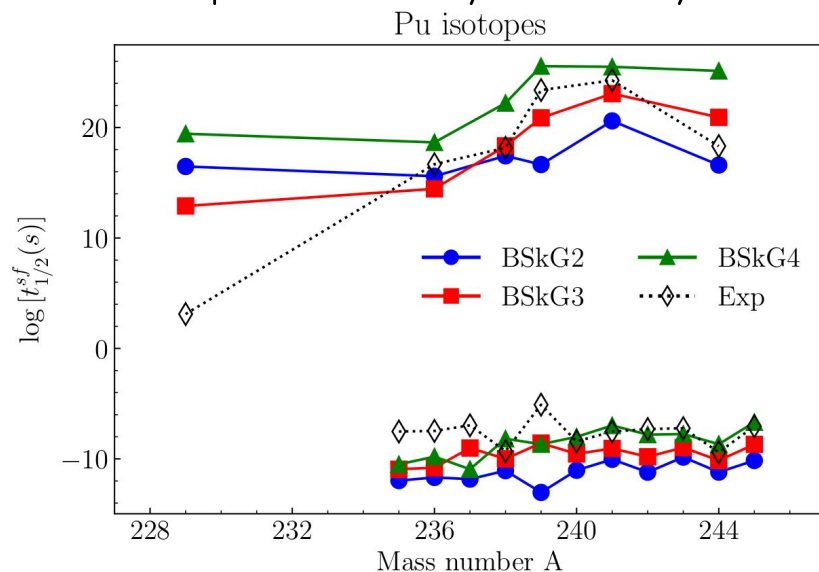
Model dependency and systematics



Model dependency

- BSkG3 is spectacular, BSkG2 /4 decent
- BSkG4 has weaker and more “realistic” pairing.

Model dependency and systematics



$$r_i = \frac{t_{1/2, \text{calc}}^{\text{sf}}}{t_{1/2, \text{exp}}^{\text{sf}}}$$

$$f_{\text{rms}} = \exp \left[\frac{1}{N} \sum_i (\ln r_i)^2 \right]^{1/2}, \quad f_{\text{mean}} = \exp \left[\frac{1}{N} \sum_i \ln r_i \right].$$

	f_{rms}			f_{mean}		
	BSkG2	BSkG3	BSkG4	BSkG2	BSkG3	BSkG4
all (124)	$1.8 \cdot 10^5$	$3.1 \cdot 10^3$	$3.2 \cdot 10^4$	10^{-3}	$7 \cdot 10^{-2}$	$1.5 \cdot 10^2$
even (59)	$3 \cdot 10^4$	$7.6 \cdot 10^2$	$5.2 \cdot 10^4$	$3 \cdot 10^{-2}$	1.5	$1.2 \cdot 10^3$
odd (65)	$7.6 \cdot 10^5$	$9.2 \cdot 10^3$	$2 \cdot 10^4$	10^{-4}	$4 \cdot 10^{-3}$	$2.4 \cdot 10^1$

Model dependency

- BSkG3 is spectacular, BSkG2 /4 decent
- BSkG4 has weaker and more “realistic” pairing.

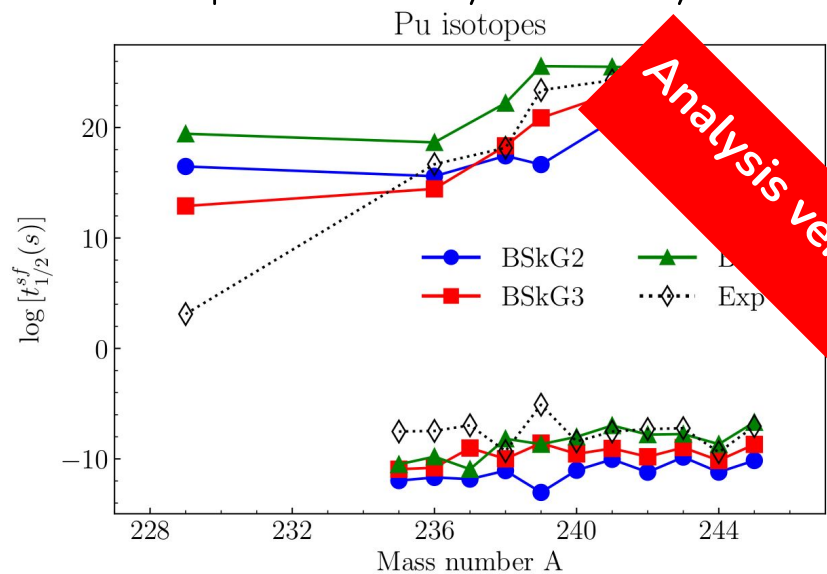
Systematics for BSkG3

- fission is too fast; mostly odds
- short half-lives underestimated
- but only ~45/124 nuclei were in the fit
- ? actual observables in the fit





Model dependency and systematics



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$3 \cdot 10^4$	$7.6 \cdot 10^2$	$5.2 \cdot 10^4$	$3 \cdot 10^{-2}$	1.5	$1.2 \cdot 10^3$
$1.1 \cdot 10^5$	$9.2 \cdot 10^3$	$2 \cdot 10^4$	10^{-4}	$4 \cdot 10^{-3}$	$2.4 \cdot 10^1$

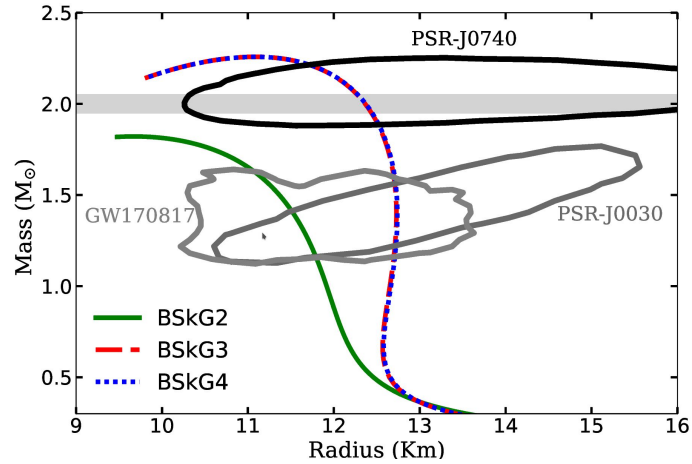
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Systematics for BSkG3

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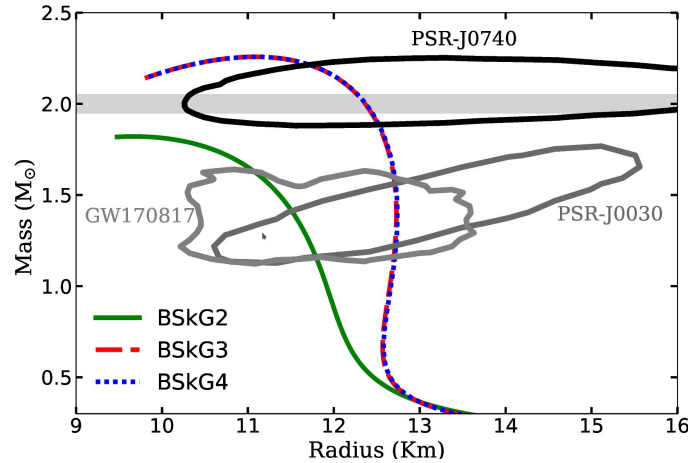
Neutron stars



Stiffer EoS

- results in higher maximum mass
- usually incompatible with masses

Neutron stars



$$\begin{aligned}
 \mathcal{E}_{t,e}(\mathbf{r}) = & C_t^{\rho\rho}(\rho_0) \rho_t^2(\mathbf{r}) + C_t^{\rho\tau}(\rho_0) \rho_t(\mathbf{r}) \tau_t(\mathbf{r}) \\
 & + C_t^{\rho\nabla J} \rho_t(\mathbf{r}) \nabla \cdot \mathbf{J}_t(\mathbf{r}) \\
 & + C_t^{\rho\Delta\rho} \rho_t(\mathbf{r}) \Delta\rho_t(\mathbf{r}) \\
 & + C_t^{\nabla\rho\nabla\rho}(\rho_0) \nabla\rho_t(\mathbf{r}) \cdot \nabla\rho_t(\mathbf{r}) \\
 & + C_t^{\rho\nabla\rho\nabla\rho}(\rho_0) \rho_t(\mathbf{r}) \nabla\rho_0(\mathbf{r}) \cdot \nabla\rho_t(\mathbf{r})
 \end{aligned}$$

Stiffer EoS

- results in higher maximum mass
- usually incompatible with masses

Extended density dependencies

- ad-hoc suggestion
 - 6 additional parameters
- ... two are fractional powers!



$$\begin{aligned}
\mathcal{E}_{\text{Sk,e}}^{(0)}(\vec{r}) &= \sum_{t=0,1} \left[A_{t,e}^{(0,1)} \left(D_t^{1,1} \right)^2 + A_{t,e}^{(0,2)} \left(D_0^{1,1} \right)^\alpha \left(D_t^{1,1} \right)^2 \right], \\
\mathcal{E}_{\text{Sk,e}}^{(2)}(\vec{r}) &= \sum_{t=0,1} \left[A_{t,e}^{(2,1)} D_t^{1,1} \left(\Delta D_t^{1,1} \right) + A_{t,e}^{(2,2)} D_t^{1,1} D_t^{\nabla, \nabla} + A_{t,e}^{(2,3)} \sum_{\mu\nu} C_{t,\mu\nu}^1 \nabla^\sigma C_{t,\mu\nu}^1 \nabla^\sigma + A_{t,e}^{(2,4)} D_t^{1,1} \left(\nabla \cdot C_t^1 \nabla \times \sigma \right) \right], \\
\mathcal{E}_{\text{Sk,e}}^{(4)}(\vec{r}) &= \sum_{t=0,1} \left[A_{t,e}^{(4,1)} \left(\Delta D_t^{1,1} \right) \left(\Delta D_t^{1,1} \right) + A_{t,e}^{(4,2)} D_t^{1,1} D_t^{\Delta, \Delta} + A_{t,e}^{(4,3)} D_t^{\nabla, \nabla} D_t^{\nabla, \nabla} \right. \\
&\quad + A_{t,e}^{(4,4)} \sum_{\mu\nu} D_{t,\mu\nu}^{\nabla, \nabla} D_{t,\mu\nu}^{\nabla, \nabla} + A_{t,e}^{(4,5)} \sum_{\mu\nu} D_{t,\mu\nu}^{\nabla, \nabla} \left(\nabla_\mu \nabla_\nu D_t^{1,1} \right) \\
&\quad \left. + A_{t,e}^{(4,6)} \sum_{\mu\nu} C_{t,\mu\nu}^1 \nabla^\sigma \left(\Delta C_{t,\mu\nu}^1 \nabla^\sigma \right) + A_{t,e}^{(4,7)} \sum_{\mu\nu\kappa} \left(\nabla_\mu C_{t,\mu\kappa}^1 \nabla^\sigma \right) \left(\nabla_\nu C_{t,\nu\kappa}^1 \nabla^\sigma \right) + A_{t,e}^{(4,8)} \sum_{\mu\nu} C_{t,\mu\nu}^1 \nabla^\sigma C_{t,\mu\nu}^{\Delta, \nabla \sigma} \right], \\
\mathcal{E}_{\text{Sk,o}}^{(0)}(\vec{r}) &= \sum_{t=0,1} \left[A_{t,o}^{(0,1)} \bar{D}_t^{1,\sigma} \cdot \bar{D}_t^{1,\sigma} + A_{t,o}^{(0,2)} \left(D_0^{1,1} \right)^\alpha \bar{D}_t^{1,\sigma} \cdot \bar{D}_t^{1,\sigma} \right], \\
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&\quad + A_{t,o}^{(4,4)} \sum_{\mu\nu\kappa} D_{\mu\nu\kappa}^{\nabla, \nabla} \sigma D_{\mu\nu\kappa}^{\nabla, \nabla} \sigma + A_{t,o}^{(4,5)} \sum_{\mu\nu\kappa} D_{\mu\nu\kappa}^{\nabla, \nabla} \sigma \left(\nabla_\mu \nabla_\nu D_\kappa^{1,\sigma} \right) \\
&\quad \left. + A_{t,o}^{(4,6)} \bar{C}_t^{1,\nabla} \cdot \left(\Delta \bar{C}_t^{1,\nabla} \right) + A_{t,o}^{(4,7)} \left(\nabla \cdot \bar{C}_t^{1,\nabla} \right) \left(\nabla \cdot \bar{C}_t^{1,\nabla} \right) + A_{t,o}^{(4,8)} \bar{C}_t^{1,\nabla} \cdot \bar{C}_t^{\Delta, \nabla} \right],
\end{aligned}$$

N2LO EDF

- **systematic** expansion in gradients
- next-to-next-to-leading order
- original motivation: spectroscopy
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$$\begin{aligned}
\mathcal{E}_{\text{Sk,e}}^{(0)}(\vec{r}) &= \sum_{t=0,1} \left[A_{t,e}^{(0,1)} \left(D_t^{1,1} \right)^2 + A_{t,e}^{(0,2)} \left(D_t^{1,1} \right)^\alpha \left(D_t^{1,1} \right)^2 \right], \\
\mathcal{E}_{\text{Sk,e}}^{(2)}(\vec{r}) &= \sum_{t=0,1} \left[A_{t,e}^{(2,1)} D_t^{1,1} \left(\Delta D_t^{1,1} \right) + A_{t,e}^{(2,2)} D_t^{1,1} D_t^{\nabla, \nabla} + A_{t,e}^{(2,3)} \sum_{\mu\nu} C_{t,\mu\nu}^1 \nabla^\sigma C_{t,\mu\nu}^1 \nabla^\sigma + A_{t,e}^{(2,4)} D_t^{1,1} \left(\nabla \cdot C_t^1 \nabla \times \sigma \right) \right], \\
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&\quad + A_{t,e}^{(4,4)} \sum_{\mu\nu} D_{t,\mu\nu}^{\nabla, \nabla} D_{t,\mu\nu}^{\nabla, \nabla} + A_{t,e}^{(4,5)} \sum_{\mu\nu} D_{t,\mu\nu}^{\nabla, \nabla} \left(\nabla_\mu \nabla_\nu D_t^{1,1} \right) \\
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&\quad + A_{t,o}^{(4,4)} \sum_{\mu\nu\kappa} D_{t,\mu\nu\kappa}^{\nabla, \nabla} D_{t,\mu\nu\kappa}^{\nabla, \nabla} + A_{t,o}^{(4,5)} \sum_{\mu\nu\kappa} D_{t,\mu\nu\kappa}^{\nabla, \nabla} \left(\nabla_\mu \nabla_\nu D_{t,\kappa}^{1,\sigma} \right) \\
&\quad \left. + A_{t,o}^{(4,6)} \bar{C}_t^{1,\nabla} \cdot \left(\Delta \bar{C}_t^{1,\nabla} \right) + A_{t,o}^{(4,7)} \left(\nabla \cdot \bar{C}_t^{1,\nabla} \right) \left(\nabla \cdot \bar{C}_t^{1,\nabla} \right) + A_{t,o}^{(4,8)} \bar{C}_t^{1,\nabla} \cdot \bar{C}_t^{\Delta, \nabla} \right],
\end{aligned}$$

N2LO EDF

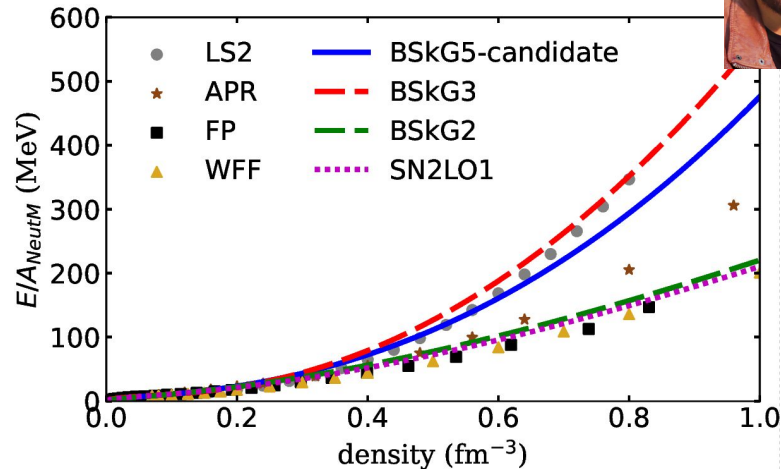
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... what if we improve INM first?



BSkG5

$$\begin{aligned}
 \mathcal{E}_{\text{Sk},e}^{(0)}(\vec{r}) &= \sum_{t=0,1} \left[A_{t,e}^{(0,1)} \left(D_t^{1,1} \right)^2 + A_{t,e}^{(0,2)} \left(D_0^{1,1} \right)^\alpha \left(D_t^{1,1} \right)^2 \right], \\
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 &\quad + A_{t,e}^{(4,4)} \sum_{\mu\nu} D_{t,\mu\nu}^{\nabla, \nabla} D_{t,\mu\nu}^{\nabla, \nabla} + A_{t,e}^{(4,5)} \sum_{\mu\nu} D_{t,\mu\nu}^{\nabla, \nabla} \left(\nabla_\mu \nabla_\nu D_t^{1,1} \right) \\
 &\quad \left. + A_{t,e}^{(4,6)} \sum_{\mu\nu} C_{t,\mu\nu}^1 \nabla^\sigma \left(\Delta C_{t,\mu\nu}^1 \nabla^\sigma \right) + A_{t,e}^{(4,7)} \sum_{\mu\nu\kappa} \left(\nabla_\mu C_{t,\mu\nu}^1 \nabla^\sigma \right) \left(\nabla_\nu C_{t,\nu\kappa}^1 \nabla^\sigma \right) + A_{t,e}^{(4,8)} \sum_{\mu\nu} C_{t,\mu\nu}^1 \nabla^\sigma C_{t,\mu\nu}^1 \Delta \nabla^\sigma \right], \\
 \mathcal{E}_{\text{Sk},o}^{(0)}(\vec{r}) &= \sum_{t=0,1} \left[A_{t,o}^{(0,1)} \vec{B}_t^{1,\sigma} \cdot \vec{B}_t^{1,\sigma} + A_{t,o}^{(0,2)} \left(D_0^{1,1} \right)^\alpha \vec{B}_t^{1,\sigma} \cdot \vec{B}_t^{1,\sigma} \right], \\
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 \end{aligned}$$

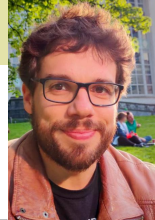


N2LO EDF

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... what if we improve INM first?

- same global quality as BSkG4
- density dependence as standard Skyrme



$$\begin{aligned}
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\mathcal{E}_{\text{Sk,e}}^{(4)}(\vec{r}) &= \sum_{t=0,1} \left[A_{t,e}^{(4,1)} \left(\Delta D_t^{1,1} \right) \left(\Delta D_t^{1,1} \right) + A_{t,e}^{(4,2)} D_t^{1,1} D_t^{\Delta, \Delta} + A_{t,e}^{(4,3)} D_t^{\nabla, \nabla} D_t^{\nabla, \nabla} \right. \\
&\quad + A_{t,e}^{(4,4)} \sum_{\mu\nu} D_{t, \mu\nu}^{\nabla, \nabla} D_{t, \mu\nu}^{\nabla, \nabla} + A_{t,e}^{(4,5)} \sum_{\mu\nu} D_{t, \mu\nu}^{\nabla, \nabla} \left(\nabla_\mu \nabla_\nu D_t^{1,1} \right) \\
&\quad \left. + A_{t,e}^{(4,6)} \sum_{\mu\nu} C_{t, \mu\nu}^{1, \nabla \sigma} \left(\Delta C_{t, \mu\nu}^{1, \nabla \sigma} \right) + A_{t,e}^{(4,7)} \sum_{\mu\nu\kappa} \left(\nabla_\mu C_{t, \mu\nu}^{1, \nabla \sigma} \right) \left(\nabla_\nu C_{t, \nu\kappa}^{1, \nabla \sigma} \right) + A_{t,e}^{(4,8)} \sum_{\mu\nu} C_{t, \mu\nu}^{1, \nabla \sigma} C_{t, \mu\nu}^{\Delta, \nabla \sigma} \right], \\
\mathcal{E}_{\text{Sk,o}}^{(0)}(\vec{r}) &= \sum_{t=0,1} \left[A_{t,o}^{(0,1)} \bar{D}_t^{1, \sigma} \cdot \bar{D}_t^{1, \sigma} + A_{t,o}^{(0,2)} \left(D_0^{1,1} \right)^\alpha \bar{D}_t^{1, \sigma} \cdot \bar{D}_t^{1, \sigma} \right], \\
\mathcal{E}_{\text{Sk,o}}^{(2)}(\vec{r}) &= \sum_{t=0,1} \left[A_{t,o}^{(2,1)} \bar{D}_t^{1, \sigma} \cdot \left(\Delta \bar{D}_t^{1, \sigma} \right) + A_{t,o}^{(2,2)} \bar{D}_t^{1, \sigma} \cdot \bar{D}_t^{\nabla, \nabla} + A_{t,o}^{(2,3)} \bar{C}_t^{1, \nabla} \cdot \bar{C}_t^{1, \nabla} + A_{t,o}^{(2,4)} \bar{D}_t^{1, \sigma} \cdot \left(\nabla \times \bar{C}_t^{1, \nabla} \right) \right], \\
\mathcal{E}_{\text{Sk,o}}^{(4)}(\vec{r}) &= \sum_{t=0,1} \left[A_{t,o}^{(4,1)} \left(\Delta \bar{D}_t^{1, \sigma} \right) \cdot \left(\Delta \bar{D}_t^{1, \sigma} \right) + A_{t,o}^{(4,2)} \bar{D}_t^{1, \sigma} \cdot \bar{D}_t^{\Delta, \Delta} + A_{t,o}^{(4,3)} \bar{D}_t^{\nabla, \nabla} \cdot \bar{D}_t^{\nabla, \nabla} \right. \\
&\quad + A_{t,o}^{(4,4)} \sum_{\mu\nu\kappa} D_{t, \mu\nu}^{\nabla, \nabla} D_{t, \mu\nu}^{\nabla, \nabla} + A_{t,o}^{(4,5)} \sum_{\mu\nu\kappa} D_{t, \mu\nu}^{\nabla, \nabla} \left(\nabla_\mu \nabla_\nu D_{t, \kappa}^{1, \sigma} \right) \\
&\quad \left. + A_{t,o}^{(4,6)} \bar{C}_t^{1, \nabla} \cdot \left(\Delta \bar{C}_t^{1, \nabla} \right) + A_{t,o}^{(4,7)} \left(\nabla \cdot \bar{C}_t^{1, \nabla} \right) \left(\nabla \cdot \bar{C}_t^{1, \nabla} \right) + A_{t,o}^{(4,8)} \bar{C}_t^{1, \nabla} \cdot \bar{C}_t^{\Delta, \nabla} \right],
\end{aligned}$$

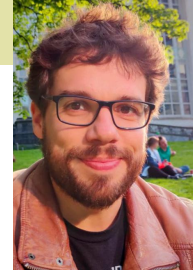
Rms σ	BSkG4	BSkG5
Masses [MeV]	0.633	0.637
S_n [MeV]	0.402	0.407
Radii [fm]	0.025	0.028
Prim. barriers [MeV]	0.36	0.36
Sec. barriers [MeV]	0.53	0.53
Fission isomers [MeV]	0.33	0.42

N2LO EDF

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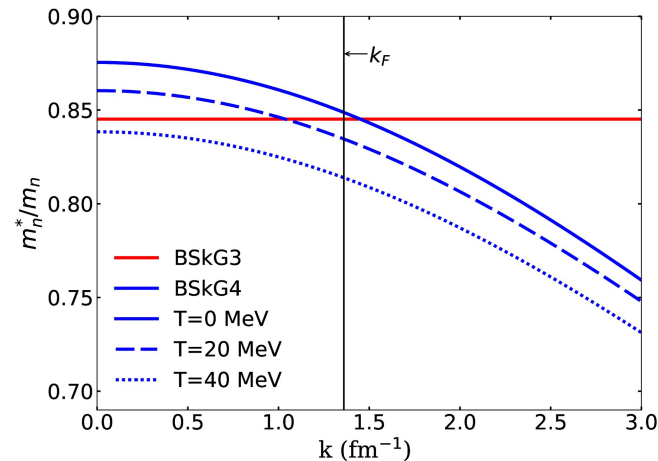
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BSkG5

$$\begin{aligned}
 \mathcal{E}_{\text{Sk},e}^{(0)}(\vec{r}) &= \sum_{t=0,1} \left[A_{t,e}^{(0,1)} \left(D_t^{1,1} \right)^2 + A_{t,e}^{(0,2)} \left(D_0^{1,1} \right)^\alpha \left(D_t^{1,1} \right)^2 \right], \\
 \mathcal{E}_{\text{Sk},e}^{(2)}(\vec{r}) &= \sum_{t=0,1} \left[A_{t,e}^{(2,1)} D_t^{1,1} \left(\Delta D_t^{1,1} \right) + A_{t,e}^{(2,2)} D_t^{1,1} D_t^{\nabla, \nabla} + A_{t,e}^{(2,3)} \sum_{\mu\nu} C_t^{1, \nabla \sigma} C_t^{1, \nabla \sigma} + A_{t,e}^{(2,4)} D_t^{1,1} \left(\nabla \cdot C_t^{1, \nabla \times \sigma} \right) \right], \\
 \mathcal{E}_{\text{Sk},e}^{(4)}(\vec{r}) &= \sum_{t=0,1} \left[A_{t,e}^{(4,1)} \left(\Delta D_t^{1,1} \right) \left(\Delta D_t^{1,1} \right) + A_{t,e}^{(4,2)} D_t^{1,1} D_t^{\Delta, \Delta} + A_{t,e}^{(4,3)} D_t^{\nabla, \nabla} D_t^{\nabla, \nabla} \right. \\
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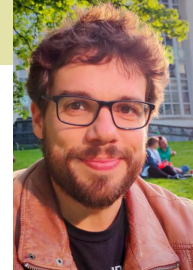


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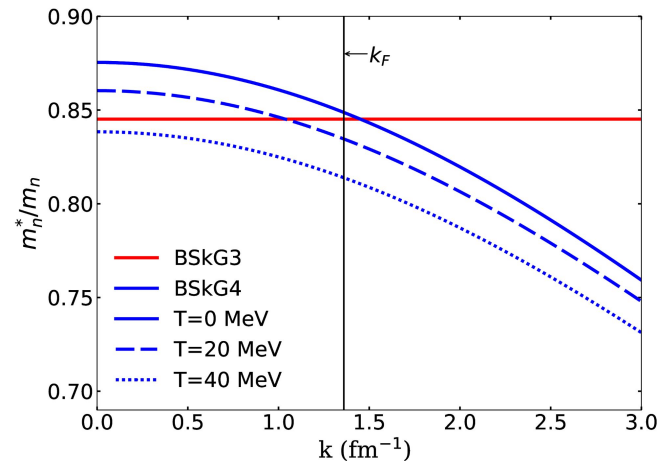
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- ... all with **LESS** parameters!

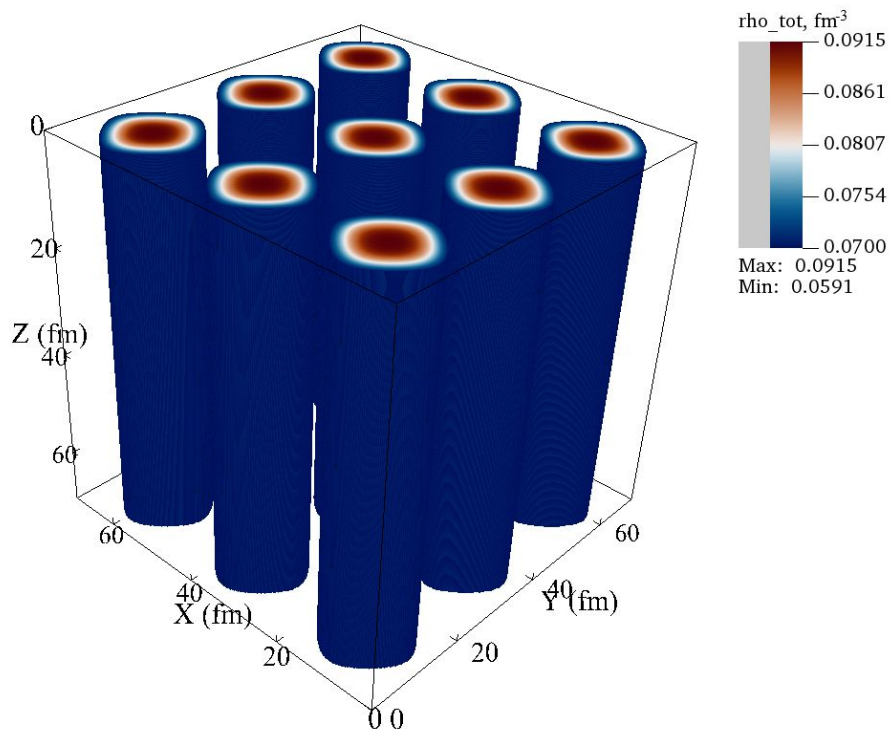
A complete EoS with the BSkGs

N. Shchechilin et al., in preparation



Nuclear pasta

- crystalline structures in NS crust
- impact NS cooling and emitted GW
- QM treatment with NS-appropriate EDFs
- $10^4 - 10^6$ particles in large volumes!

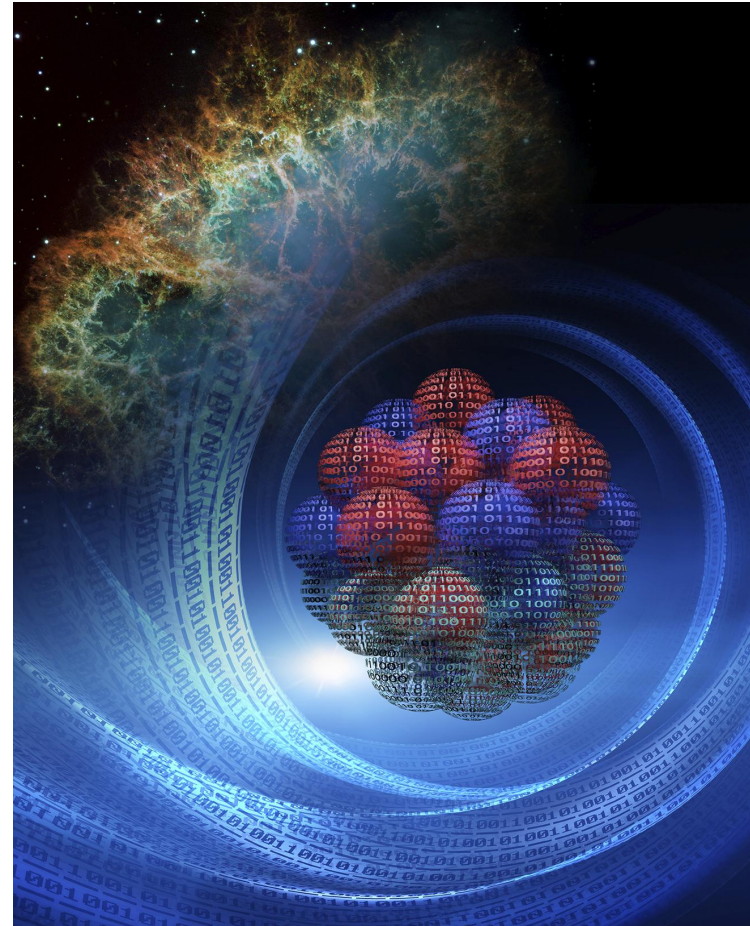


Conclusion

We build large-scale, microscopic models for (astro) applications.

Large-scale = **thousands** of nuclei and **many observables**.

Microscopic = simple wave functions yet complex **symmetry breaking**.



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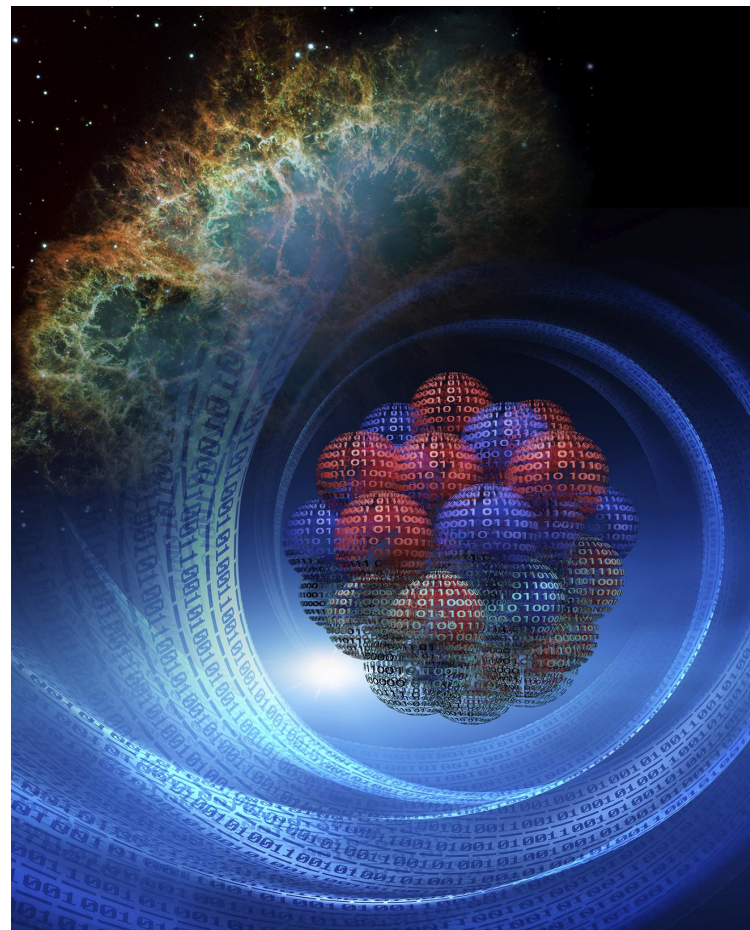
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- unmatched for fission properties
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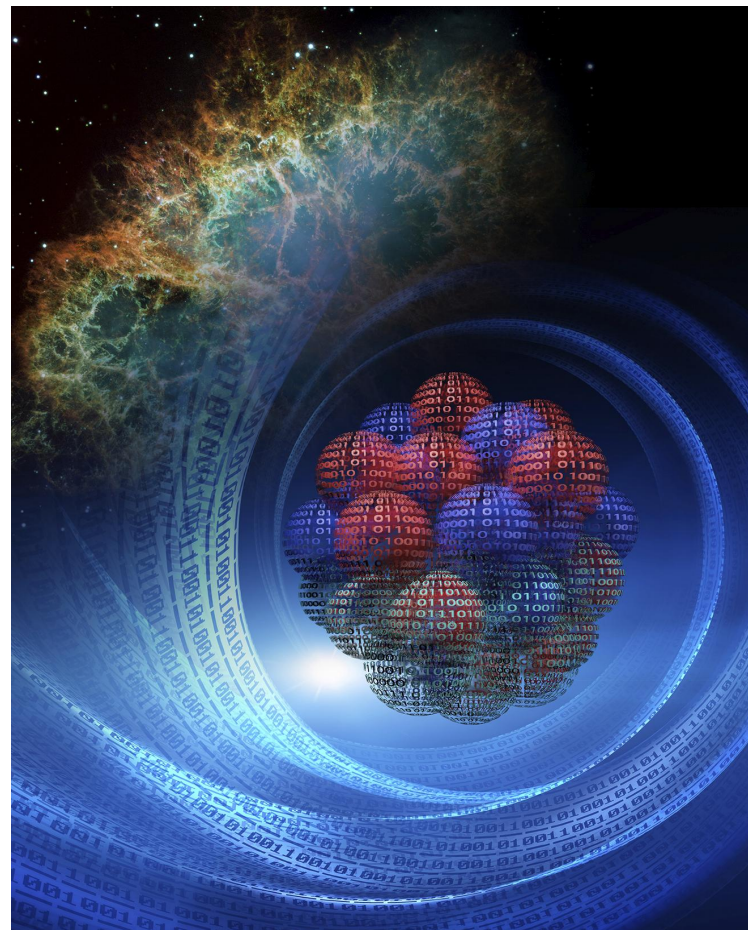
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Quite soon:

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3. a unified neutron star EoS





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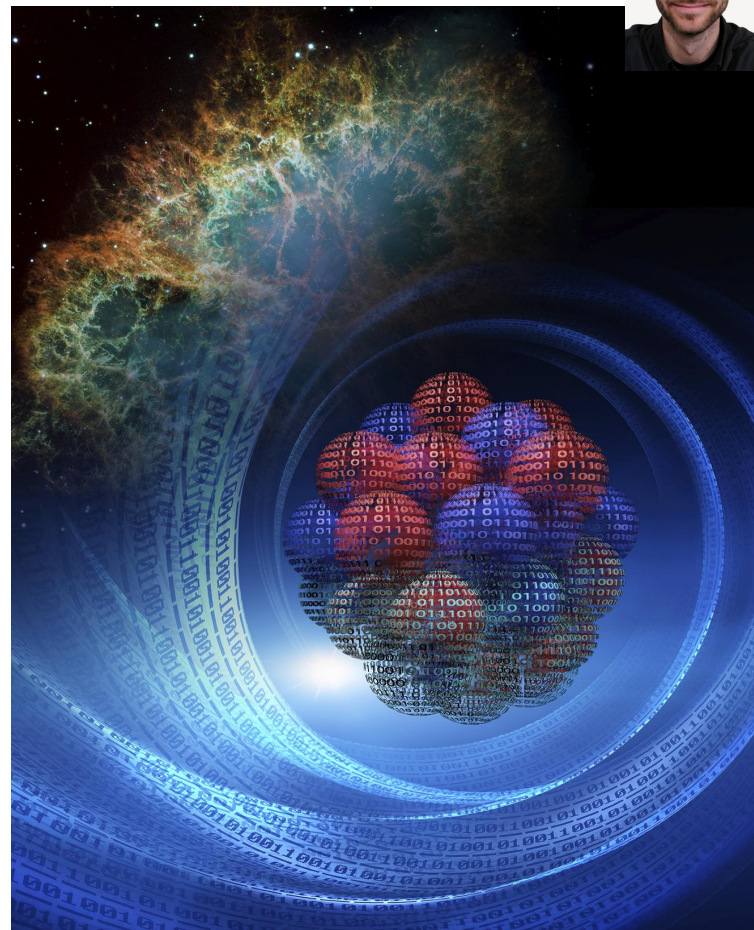
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Thank you for...

..... all the wonderful work!



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